Electronic Supplementary Material (ESI) for Chemical Communications.

Supporting Information

Contrasting Reactivity of B–Cl and B–H Bonds at [Ni(IMes)$_2$] for the Formation of Unsupported Ni-Boryls

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Contents

Experimental

General

All manipulations were carried out under an atmosphere of argon or dinitrogen using standard Schlenk line and glovebox techniques. All reactions were carried out in oven- then flame-dried glassware. Prior to use all solvents were dried and stored over activated 4 Å molecular sieves or a potassium mirror. IMes[1], $Ni(IMes)_2$[2], ClBcat[3], ClBdan[4] and HBdan[5] were prepared according to literature procedures with minor modifications. Catechol was recrystallised from toluene prior to use. All other reagents were used without further purification. NMR spectra were measured at 298 K using a Bruker Ascend 400 MHz. NMR spectra chemical shifts were reported in ppm and referenced to the residual solvent signal for ^{1}H and ^{13}C spectra for C_6D_6 (δ 7.16, 128.06). Elemental analyses were performed at the London Metropolitan University by Orla McCullough.

Synthesis

Preparation of $Ni(IMes)_2(Bcat)Cl$ (**2**)

ClBcat (0.05 g, 0.32 mmol) in toluene (2 mL) was slowly added to a stirring solution of $Ni(IMes)_2$ (0.19 g, 0.29 mmol) in toluene (10 mL). Upon complete addition, the dark purple solution decolourised to a cloudy dark yellow. The reaction mixture was filtered and the solvent removed *in vacuo* leaving a dark yellow solid. The solid was extracted into hexane (3 x 3 mL) affording a yellow-orange solution which was then filtered and stored at -30 °C for 18 h yielding pale yellow crystals. Yield 0.09 g, 40 %.

Spectroscopic data: ^{1}H NMR (400.23 MHz, C_6D_6, 25 °C): δ 6.98 (4H, s, *m*-Ar*H*), 6.83-6.81 (2H, m, Bcat Ar*H*), 6.78-6.75 (6H, m, overlapping *m*-Ar*H* and Bcat Ar*H*), 6.02 (4H, s, NC*H*), 2.39 (12H, s, CH_3), 2.36 (12H, s, CH_3), 1.72 (12H, s, CH_3). **$^{13}C\{^{1}H\}$ NMR** (100.65 MHz, C_6D_6, 25 °C): δ 187.4 (s, N*C*N), 150.0 (Bcat Ar*C*), 138.4 (Mes Ar*C*), 137.3 (Mes Ar*C*), 137.2 (Mes Ar*C*), 135.3 (Mes Ar*C*), 129.8 (s, Mes Ar*C*), 128.2 (Mes Ar*C*), 122.2 (s, N*C*H), 120.6 (Bcat Ar*C*), 110.5 (Bcat Ar*C*), 21.3 (s, *C*H_3), 20.6 (s, *C*H_3), 18.3 (s, *C*H_3). **$^{11}B\{^{1}H\}$ NMR** (128.41 MHz, C_6D_6, 25 °C): δ 37.3 (br), impurity resonance at 15.2.

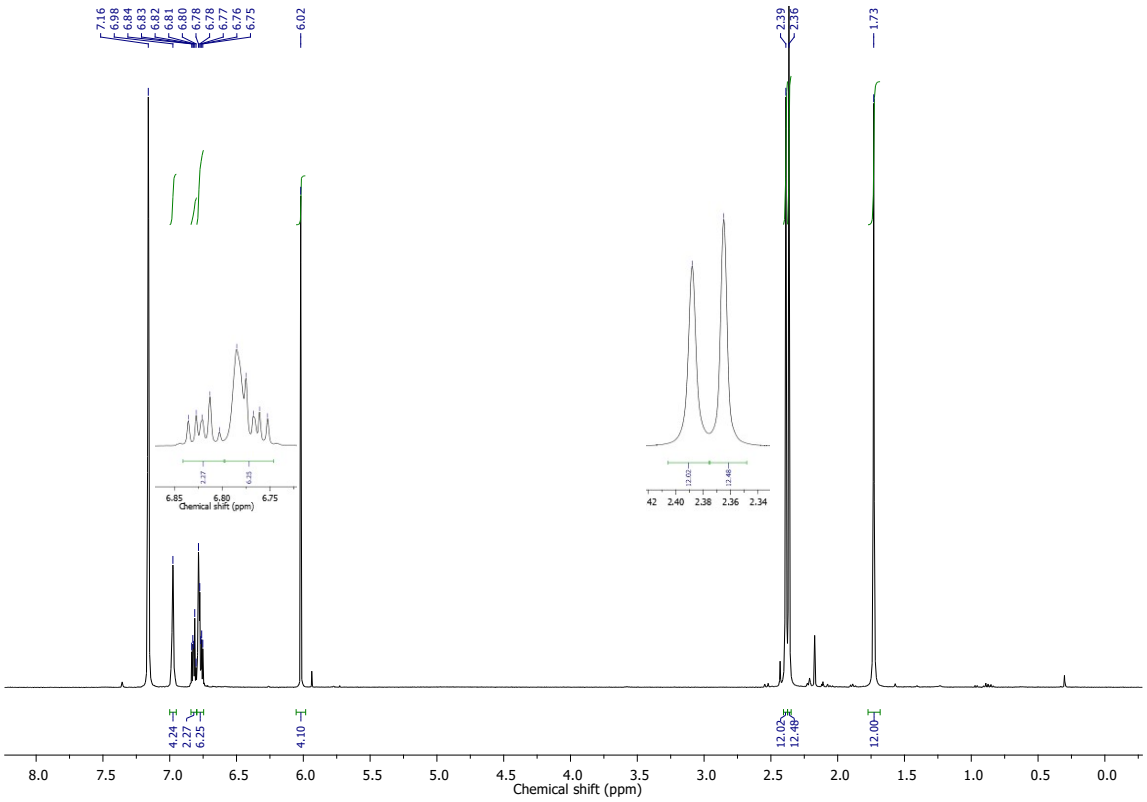


Figure S1. ^{1}H NMR spectrum (400 MHz, C_6D_6, 298 K) of Ni(IMes)$_2$(Bcat)Cl.

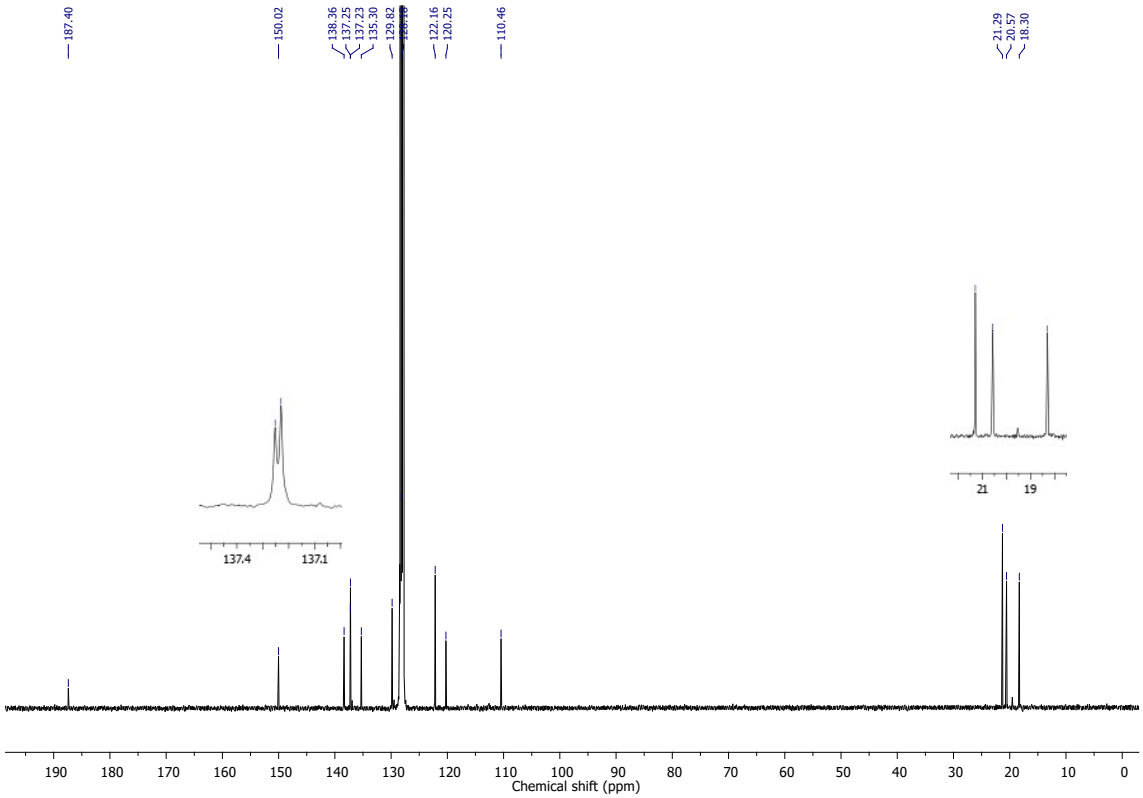


Figure S2. ^{13}C NMR spectrum (101 MHz, C_6D_6, 298 K) of Ni(IMes)$_2$(Bcat)Cl.

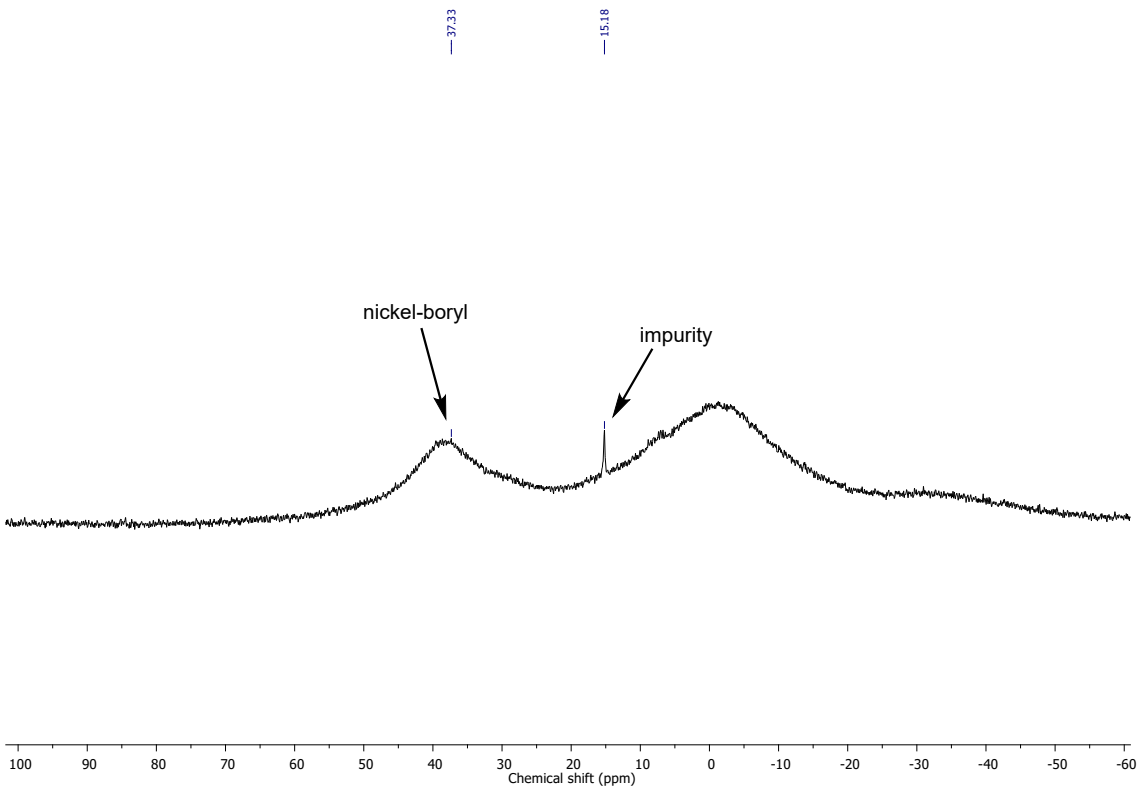


Figure S3. $^{11}B\{^{1}H\}$ NMR spectrum (128 MHz, C_6D_6, 298 K) of $Ni(IMes)_2(Bcat)Cl$.

NMR study for the ClBcat initiated decomposition of $Ni(IMes)_2(Bcat)Cl$

In a J Young's NMR tube, ClBcat (0.002 g, 0.01 mmol) was added to a solution of $Ni(IMes)_2(Bcat)Cl$ (0.008 g, 0.01 mmol) in C_6D_6. The ^{1}H and ^{11}B NMR spectra were recorded immediately and then periodically whilst maintaining room temperature.

Spectroscopic data: $^{11}B\{^{1}H\}$ NMR (128.41 MHz, C_6D_6, 25 °C): δ 37.7 (br, Ni-boryl), 28.7 (ClBcat), redistribution products (marked as *) at 22.3, 15.2, 9.3, 8.0, 6.4.

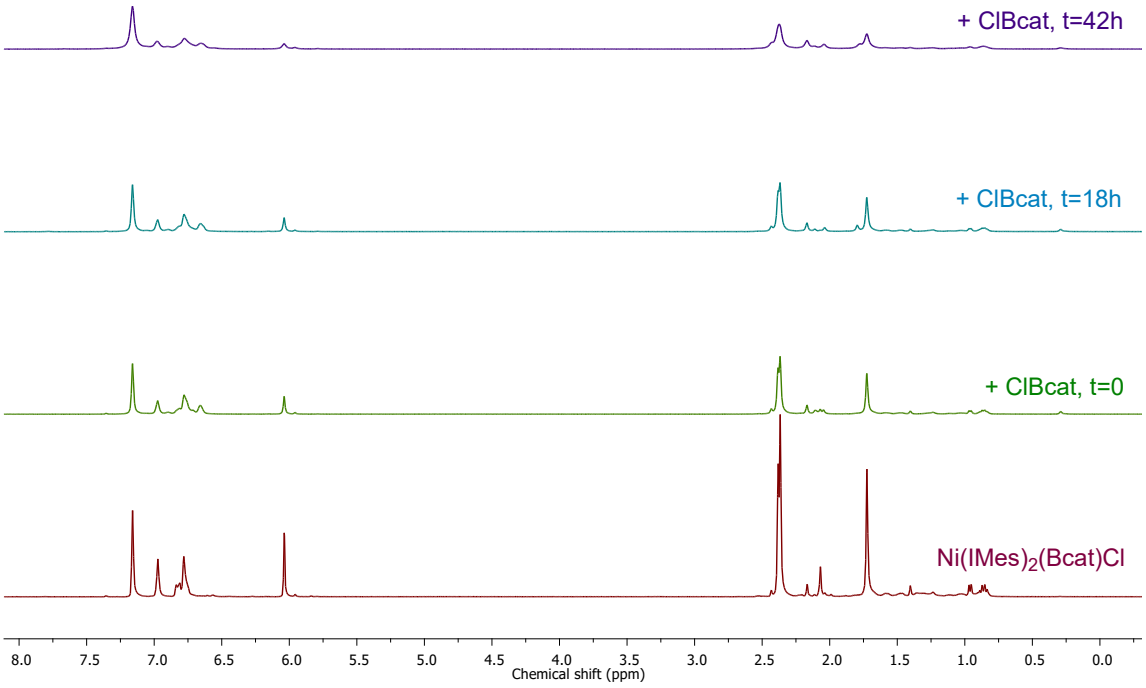


Figure S4. ^{1}H NMR spectra (400 MHz, C_6D_6, 298 K) of the addition of ClBcat to a solution of $Ni(IMes)_2(Bcat)Cl$.

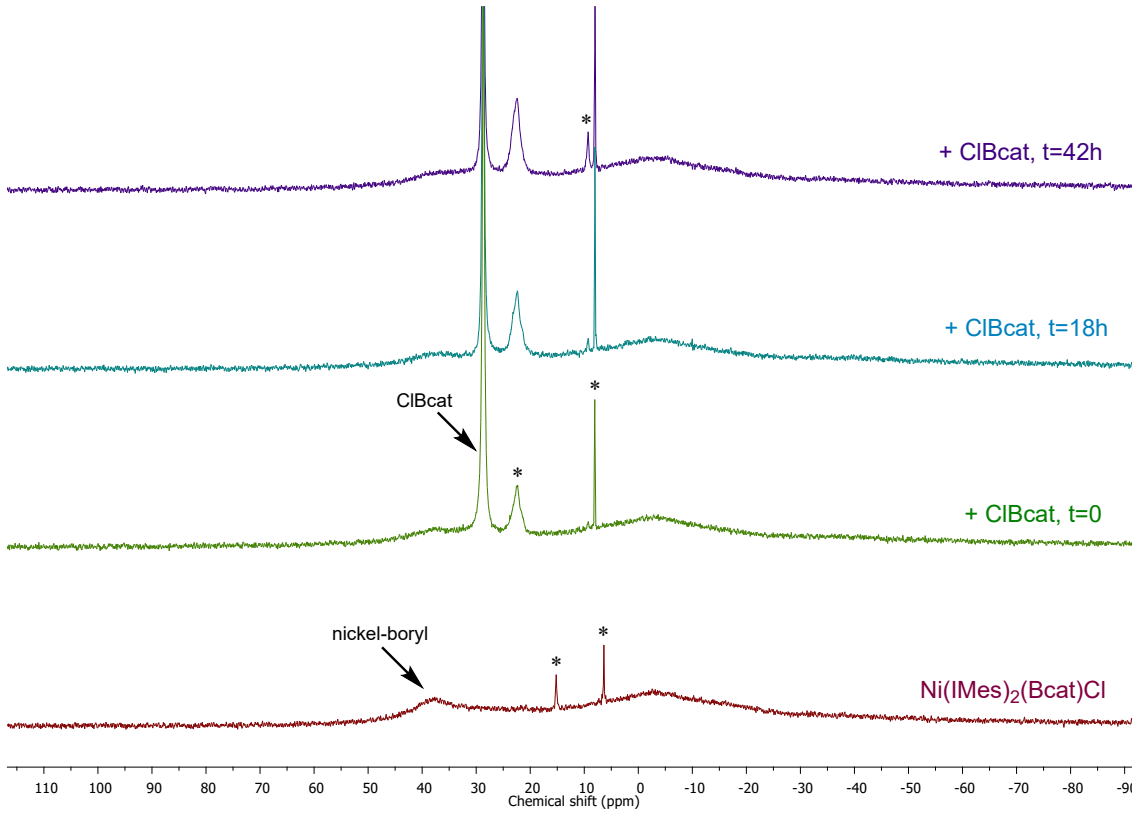


Figure S5. $^{11}B\{^{1}H\}$ NMR spectra (128 MHz, C_6D_6, 298 K) of the addition of ClBcat to a solution of $Ni(IMes)_2(Bcat)Cl$. Resonances for redistribution products are marked as *.

Preparation of Ni(IMes)$_2$(Bdan)Cl·xToluene (**3**)

A solution of ClBdan (0.15 g, 0.74 mmol) in toluene (3 mL) was added to a solution of Ni(IMes)$_2$ (0.45 g, 0.67 mmol) in toluene (12 mL). Stirring was continued for 15 min and decolourisation from dark purple to a cloudy orange was observed. The reaction mixture was filtered and the solvent removed *in vacuo* leaving a pale yellow-brown solid. The solid was redissolved in toluene (10 mL), filtered, concentrated and then stored at -20 °C for 3 days yielding pale yellow crystals. Yield 0.46 g, 79 %. Crystals suitable for SCXRD were isolated as a solvate Ni(IMes)$_2$(Bdan)Cl·0.4Toluene.

Spectroscopic data: ^{1}H NMR (400.23 MHz, C_6D_6, 25 °C): δ 7.25 (2H, m, Dan Ar*H*), 7.11 (2H, d, $^{3}J_{H\text{-}H}$ = 8.3 Hz, Dan Ar*H*), 6.87 (4H, s, *m*-Ar*H*), 6.74 (4H, s, *m*-Ar*H*), 5.97 (4H, s, NC*H*), 5.86 (2H, dd, $^{3}J_{H\text{-}H}$ = 7.3, 0.8 Hz, Dan Ar*H*), 4.64 (2H, s, CN*H*), 2.65 (12H, s, CH_3), 2.36 (12H, s, CH_3), 1.63 (12H, s, CH_3). **^{13}C{^{1}H} NMR** (100.65 MHz, C_6D_6, 25 °C): δ 190.0 (s, N*C*N), 140.7 (Dan Ar*C*), 138.3 (Mes Ar*C*), 137.4 (Mes Ar*C*), 137.2 (Dan Ar*C*), 136.0 (Mes Ar*C*), 130.0 (Mes Ar*C*), 128.2 (Mes Ar*C*), 127.9 (Mes Ar*C*), 127.7 (Dan Ar*C*), 122.6 (s, N*C*H), 118.9 (Dan Ar*C*), 116.0 (Dan Ar*C*), 103.8 (Dan Ar*C*), 21.4 (Mes *C*H$_3$), 20.9 (Mes *C*H$_3$), 18.1 (Mes *C*H$_3$). **^{11}B{^{1}H} NMR** (128.41 MHz, C_6D_6, 25 °C): δ 41.3 (br). Anal. Calcd for $C_{52}H_{56}BClN_6Ni$·0.4Toluene: C 72.58, H 6.58, N 9.27; found C 72.28, H 6.28, N 9.24.

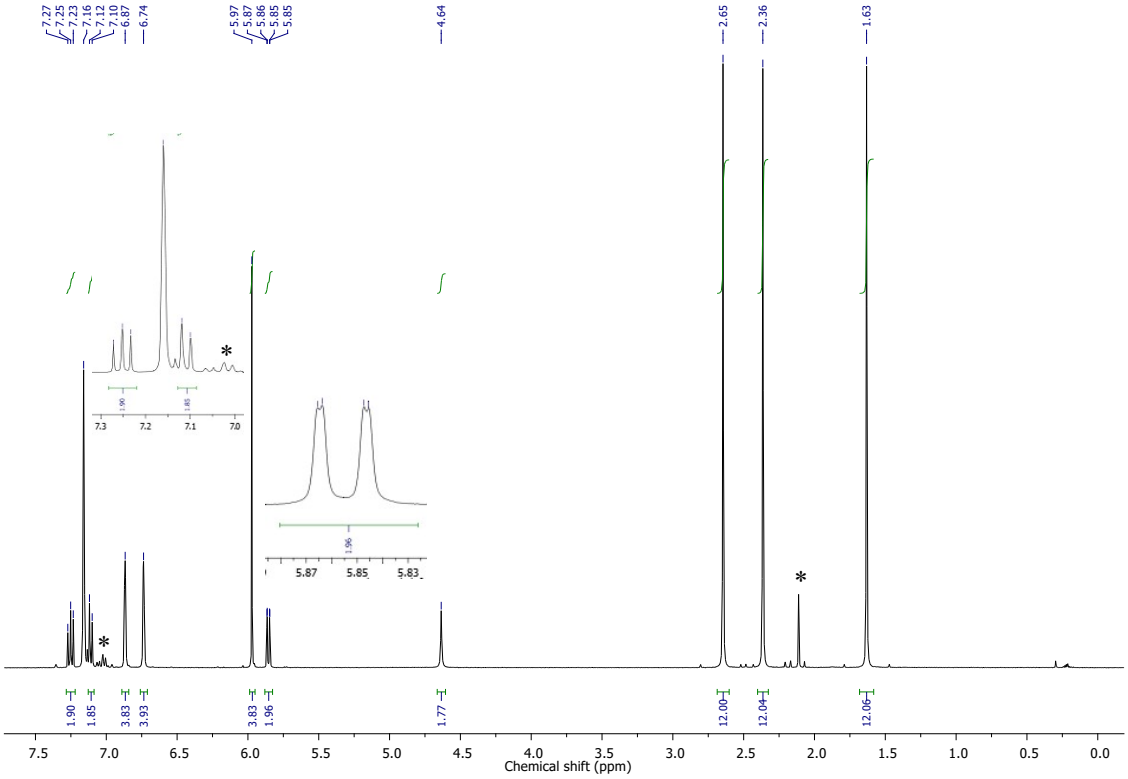


Figure S6. ^{1}H NMR spectrum (400 MHz, C_6D_6, 298 K) of Ni(IMes)$_2$(Bdan)Cl. Resonances for toluene are marked as *.

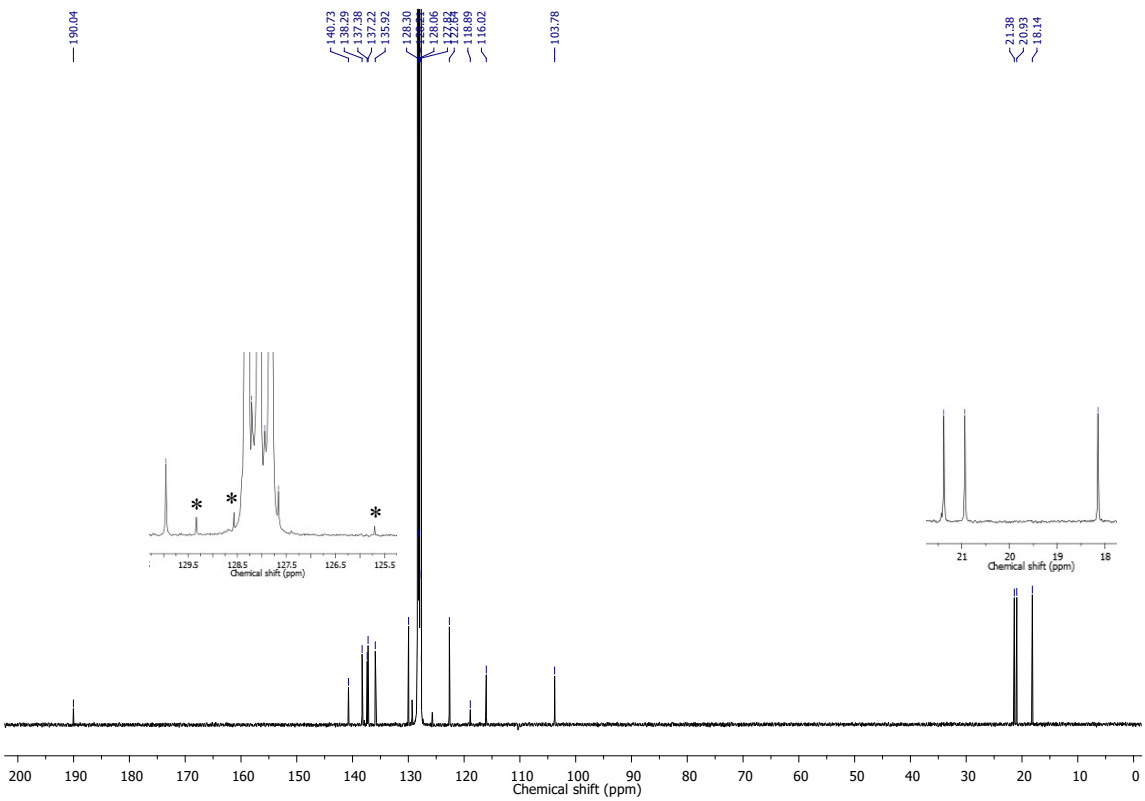


Figure S7. ^{13}C NMR spectrum (101 MHz, C_6D_6, 298 K) of Ni(IMes)$_2$(Bdan)Cl. Resonances for toluene are marked as *.

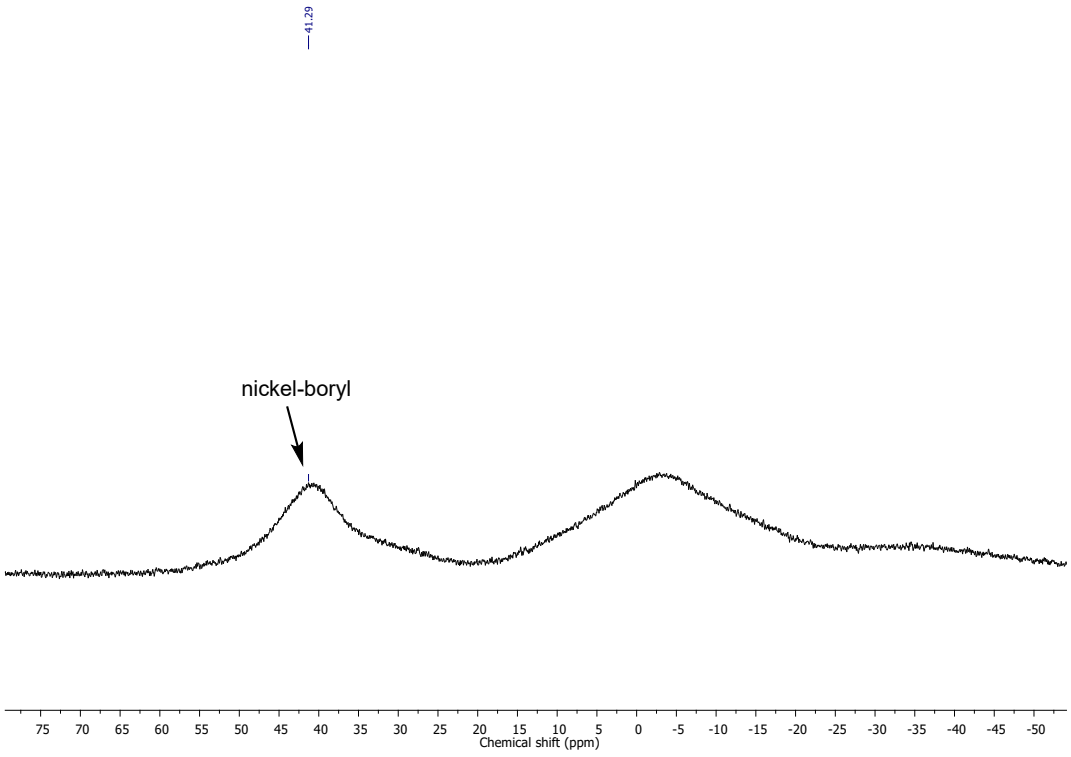


Figure S8. $^{11}B\{^1H\}$ NMR spectrum (128 MHz, C_6D_6, 298 K) of Ni(IMes)$_2$(Bdan)Cl.

Preparation of Ni(IMes)$_2$(Bdan)Me·xEt$_2$O (**5**)

MeLi (0.18 mL, 1.6 M in Et_2O, 0.29 mmol) was added dropwise to a solution of Ni(IMes)$_2$(Bdan)Cl (0.23 g, 0.26 mmol) in toluene (15 mL) at -78 °C. Stirring was continued at -78 °C for 1 h, after which the cold bath was removed and the cloudy yellow reaction mixture was filtered and the solvents removed *in vacuo*. The solid was redissolved in Et_2O (10 mL) and the cloudy orange reaction mixture was filtered, concentrated and stored at -20 °C yielding bright yellow crystals. Yield 0.13 g, 59 %. Crystals suitable for SCXRD were isolated as Ni(IMes)$_2$(Bdan)Me.0.5Et_2O.

Spectroscopic data: ^{1}H NMR (400.23 MHz, C_6D_6, 25 °C): δ 7.29 (2H, dd, $^3J_{H-H}$ = 8.2, 0.8 Hz, Dan Ar*H*), 7.12 (2H, dd, $^3J_{H-H}$ = 8.2, 0.7 Hz, Dan Ar*H*), 6.79 (4H, s, *m*-Ar*H*), 6.77 (4H, s, *m*-Ar*H*), 6.03 (4H, s, NC*H*), 5.85 (2H, dd, $^3J_{H-H}$ = 7.3, 0.8 Hz, Dan Ar*H*), 4.77 (2H, s, br, CN*H*), 2.35 (12H, s, CH_3), 2.26 (12H, s, CH_3), 1.77 (12H, s, CH_3), -0.75 (3H, s, Ni-CH_3). **^{13}C{^{1}H} NMR** (100.65 MHz, C_6D_6, 25 °C): δ 201.8 (s, N*C*N), 141.3 (Dan Ar*C*), 138.1 (Mes Ar*C*), 136.8 (Mes Ar*C*), 136.6 (Mes Ar*C*), 129.3 (Mes Ar*C*), 128.7 (Mes Ar*C*), 128.2 (Mes Ar*C*), 127.9 (Dan Ar*C*), 127.7 (Dan Ar*C*), 122.2 (s, N*C*H), 119.2 (Dan Ar*C*), 115.1 (Dan Ar*C*), 103.4 (Dan Ar*C*), 21.3 (Mes *C*H$_3$), 19.9 (Mes *C*H$_3$), 18.5 (Mes *C*H$_3$), 2.5 (s, Ni-*C*H$_3$). **^{11}B{^{1}H} NMR** (128.41 MHz, C_6D_6, 25 °C): δ 49.5 (br). Anal. Calcd for $C_{53}H_{59}BN_6Ni·0.5Et_2O$: C 74.50, H 7.28, N 9.48; found C 74.10, H 7.17, N 9.27.

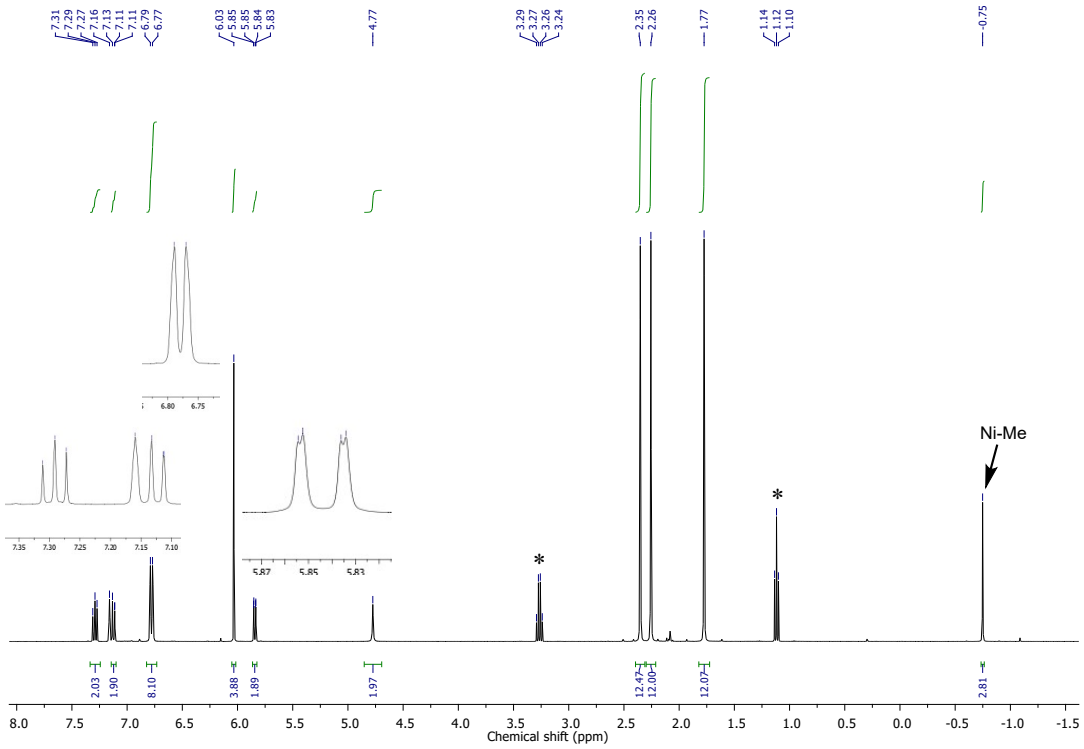


Figure S9. ^{1}H NMR spectrum (400 MHz, C_6D_6, 298 K) of Ni(IMes)$_2$(Bdan)Me. Resonances for diethyl ether are marked as *.

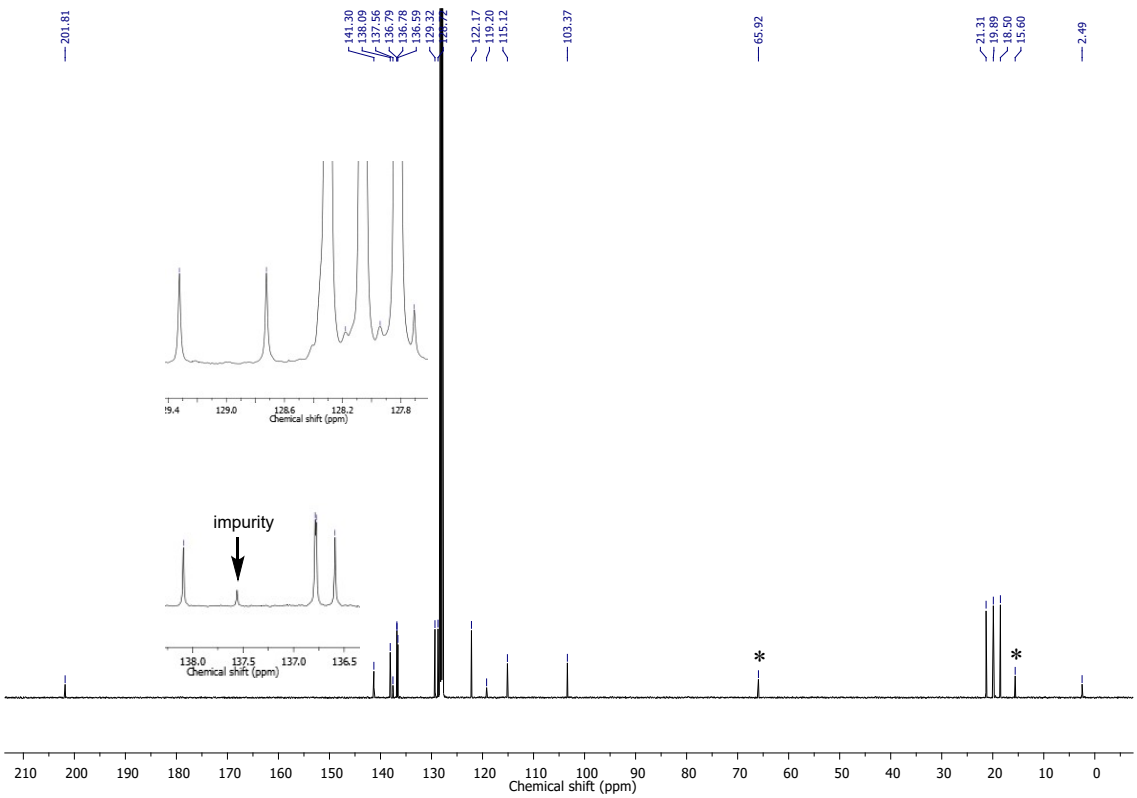


Figure S10. ^{13}C NMR spectrum (101 MHz, C_6D_6, 298 K) of Ni(IMes)$_2$(Bdan)Me. Resonances for diethyl ether are marked as *.

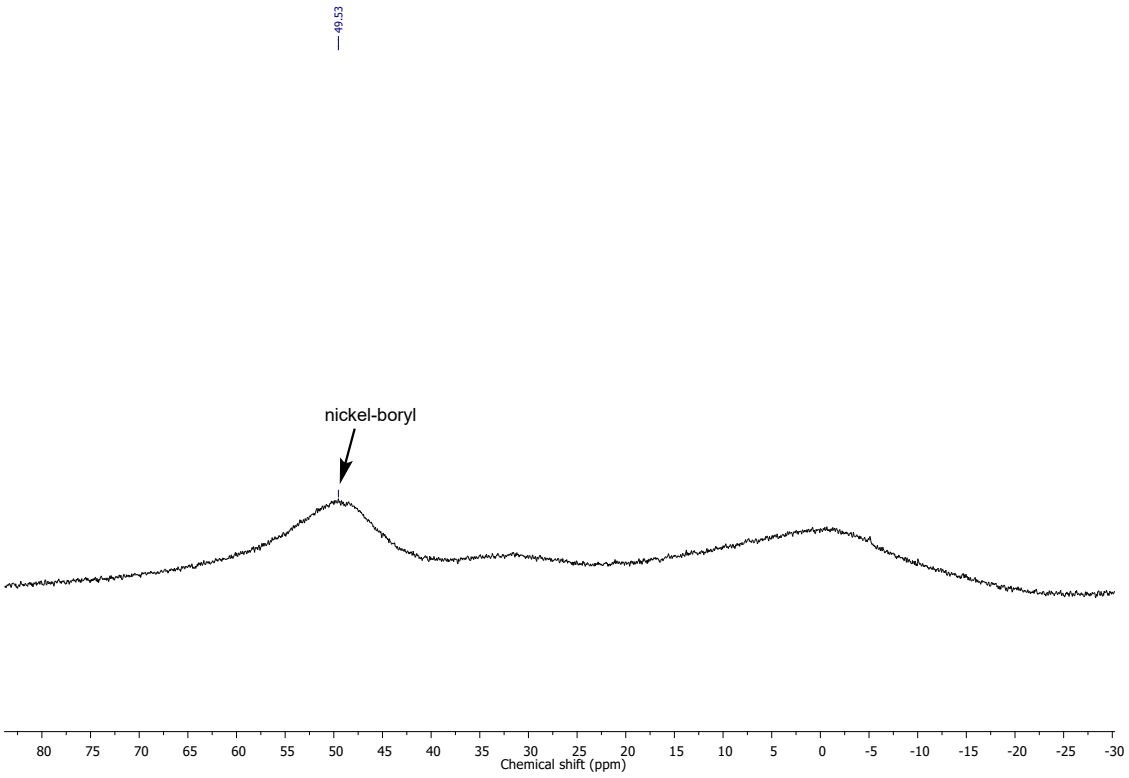


Figure S11. $^{11}B\{^1H\}$ NMR spectrum (128 MHz, C_6D_6, 298 K) of Ni(IMes)$_2$(Bdan)Me.

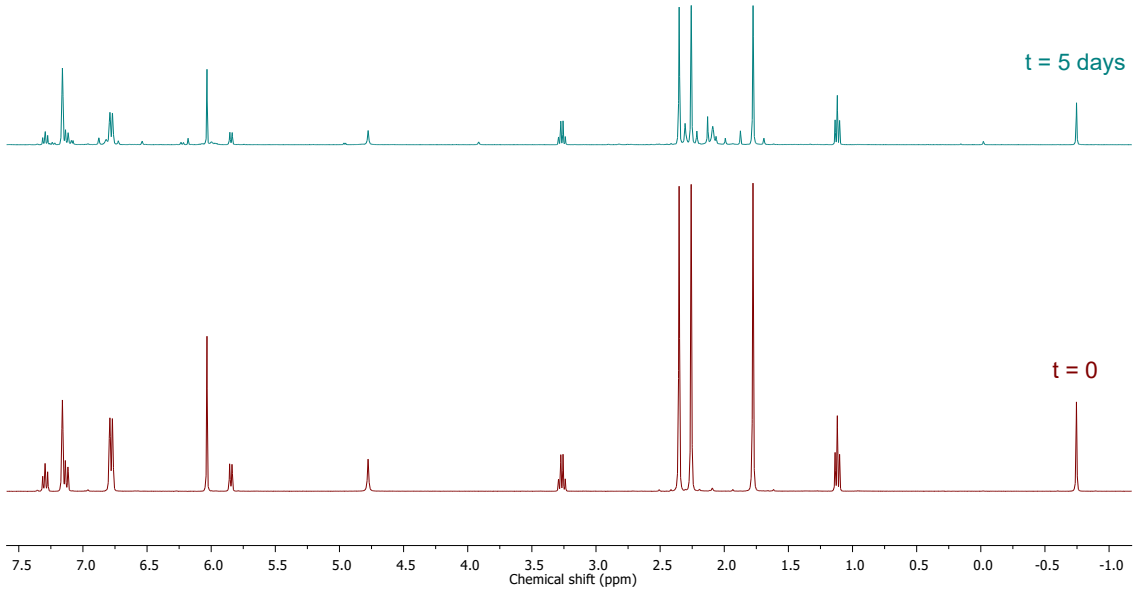


Figure S12. ^{1}H NMR spectrum (400 MHz, C_6D_6, 298 K) of Ni(IMes)$_2$(Bdan)Me (**5**) at t = 0 and t = 5 days.

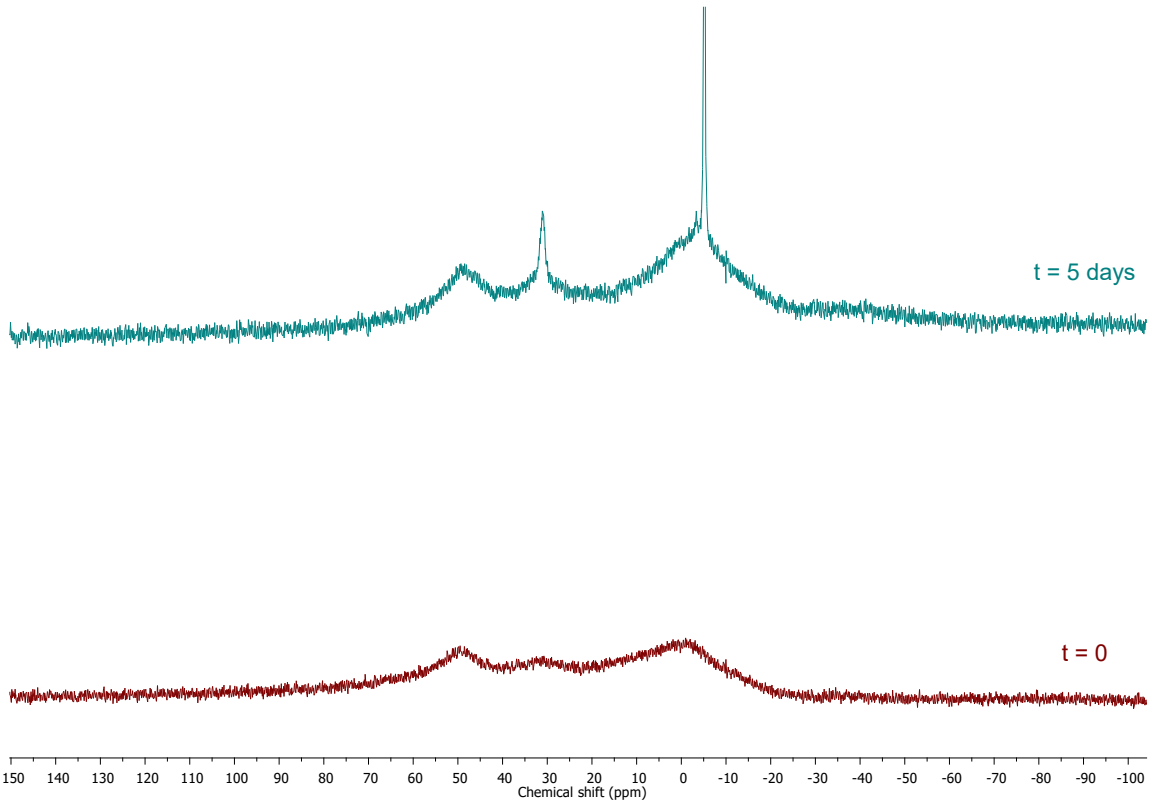


Figure S13. ^{11}B{^{1}H} NMR spectrum (128 MHz, C_6D_6, 298 K) of Ni(IMes)$_2$(Bdan)Me (**5**) at t = 0 and t = 5 days.

Preparation of Ni(IMes)$_2$(Bdan)H (**4**)

Na[HBEt$_3$] (0.32 mL, 1.0 M in THF, 0.32 mmol) was added dropwise to a solution of Ni(IMes)$_2$(Bdan)Cl (0.27 g, 0.31 mmol) in toluene (15 mL) at -78 °C. An immediate colour change from dark yellow to brown was observed. Stirring was continued for a further 30 min at -78 °C and then the reaction mixture was filtered whilst maintaining a temperature of -30 °C. Solvents were removed *in vacuo* and the solid was redissolved in toluene (10 mL) and filtered (attempting to keep both the reaction mixture and the filtrate as cool as possible with use of the glovebox freezer at -30 °C). The orange-brown solution was concentrated and stored at -20 °C yielding pale brown-grey crystals. Yield 0.13 g, 51 %.

Spectroscopic data: ^{1}H NMR (400.23 MHz, C_6D_6, 25 °C): δ 7.29-7.25 (2H, m, Ar*H*), 7.13-7.10 (2H, m, Ar*H*), 6.77 (8H, s, *m*-Ar*H*), 6.04 (4H, s, NC*H*), 5.90 (2H, dd, $^3J_{H\text{-}H}$ = 7.3, 0.8 Hz, Ar*H*), 4.65 (2H, s, CN*H*), 2.35 (12H, s, CH_3), 2.05 (24H, s, CH_3), -4.62 (1H, s, Ni-H). **^{13}C{^{1}H} NMR** (100.65 MHz, C_6D_6, 25 °C): δ 199.1 (N*C*N), 141.3 (Dan Ar*C*), 137.7 (Dan Ar*C* overlapping with Mes Ar*C*), 136.8 (Mes Ar*C*), 136.7 (Mes Ar*C*), 128.9 (Mes Ar*C*), 127.9 (Dan Ar*C*), 120.7 (N*C*H), 119.4 (Dan Ar*C*), 115.2 (Dan Ar*C*), 103.2 (Dan Ar*C*), 21.4 (Mes CH_3), 18.8 (Mes *C*H_3). **^{11}B{^{1}H} NMR** (128.41 MHz, C_6D_6, 25 °C): δ 50.0 (br), decomposition product at -12.4. Due to high air/moisture and thermal sensitivity, successful elemental analysis could not be obtained.

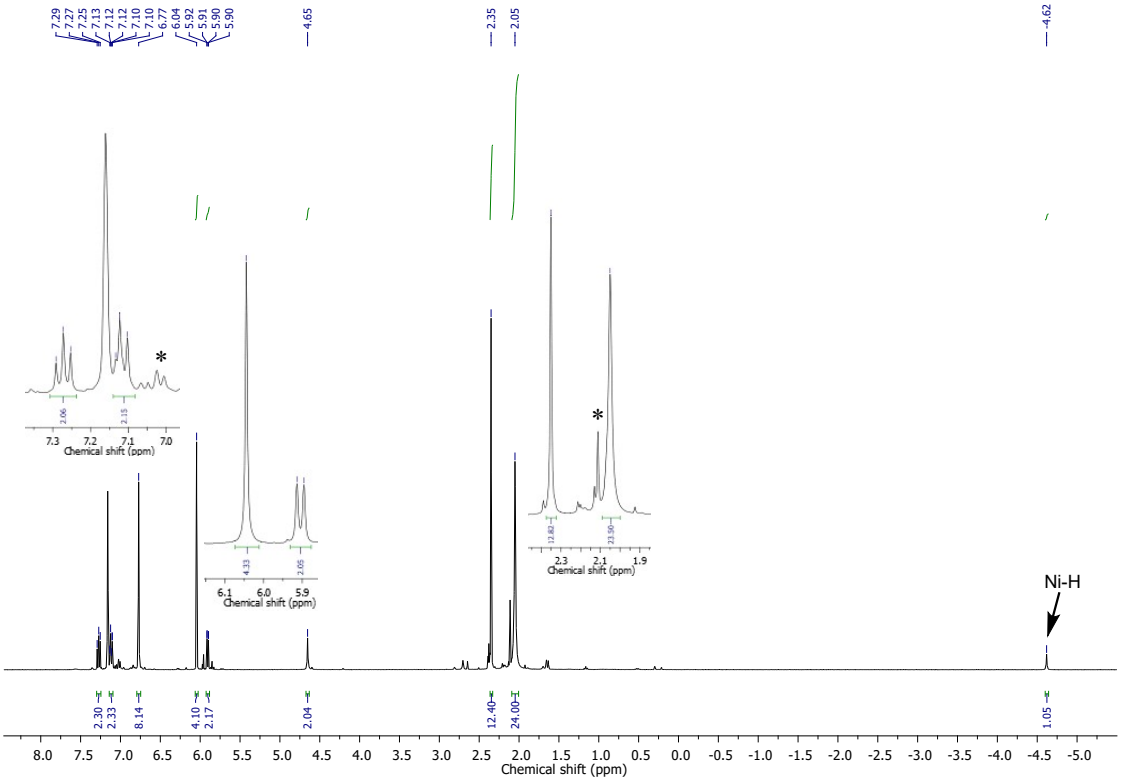


Figure S14. ^{1}H NMR spectrum (400 MHz, C_6D_6, 298 K) of Ni(IMes)$_2$(Bdan)H. Resonances for toluene are marked as *.

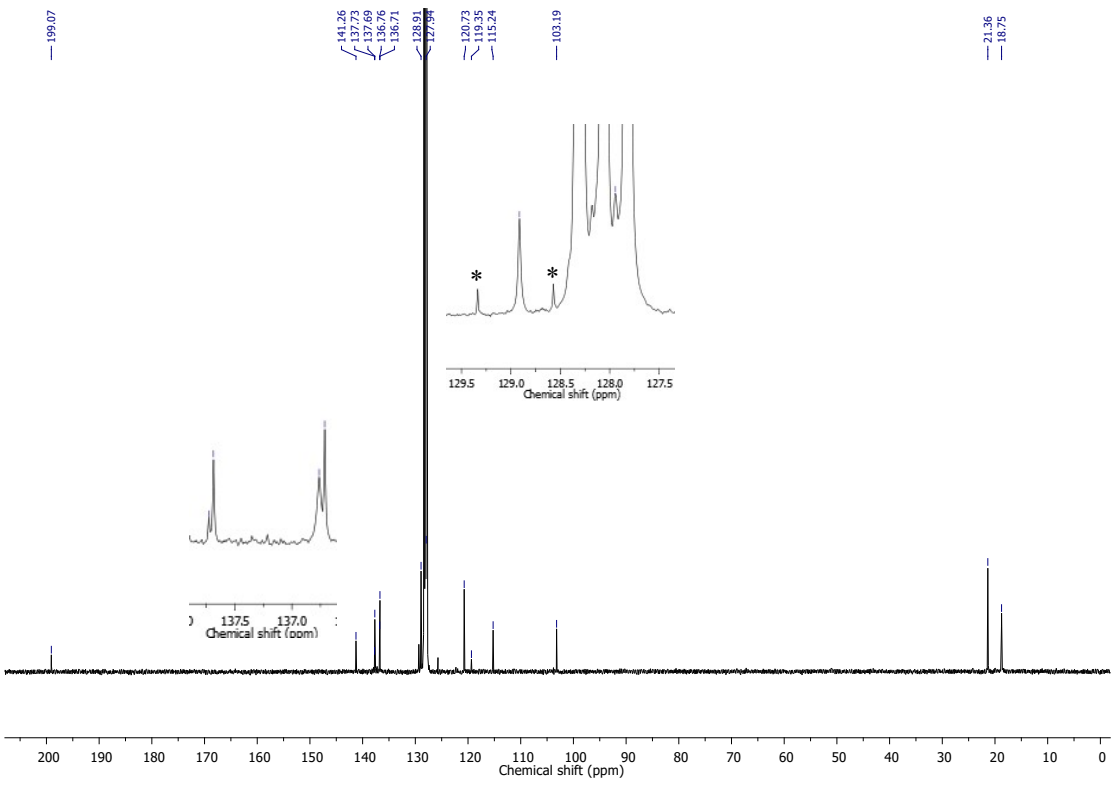


Figure S15. ^{13}C NMR spectrum (101 MHz, C_6D_6, 298 K) of $Ni(IMes)_2(Bdan)H$. Resonances for toluene are marked as *.

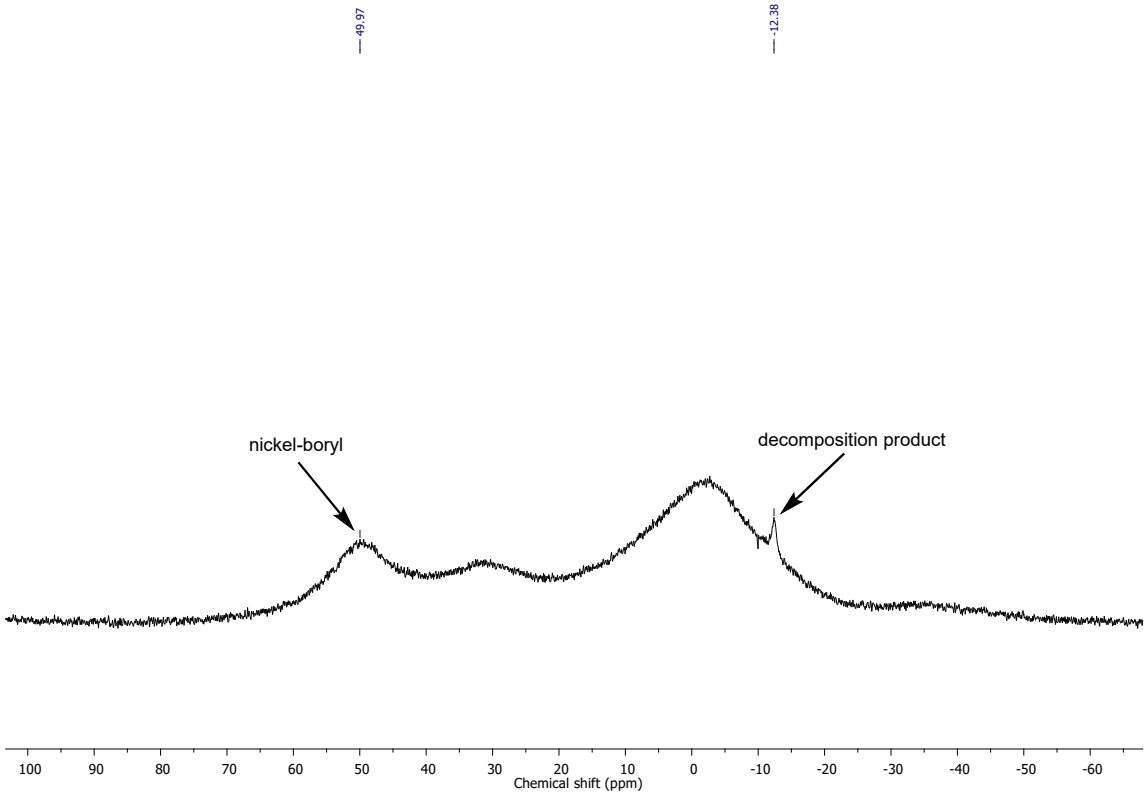


Figure S16. $^{11}B\{^1H\}$ NMR spectrum (128 MHz, C_6D_6, 298 K) of $Ni(IMes)_2(Bdan)H$.

Reaction between Ni(IMes)$_2$ and HBdan in C_6D_6

In a J Young's NMR tube, Ni(IMes)$_2$ (20 mg, 0.030 mmol) was added to a solution of HBdan (5 mg, 0.030 mmol) in C_6D_6. A dark purple solution was observed. The ^{1}H and ^{11}B NMR spectra were recorded immediately, after 1 day and after 7 days whilst maintaining room temperature. At 7 days, a black solution alongside a crystalline solid was observed in the tube. The colourless crystals were characterized by single crystal X-ray diffraction as the product of dehydrocoupling IMes.HBdanBdan.

Reaction between Ni(IMes)$_2$ and HBcat in C_6D_6

In a J Young's NMR tube, HBcat (2 μL, 0.021 mmol) was added to a solution of Ni(IMes)$_2$ (14 mg, 0.021 mmol) in C_6D_6. A colour change from dark purple to dark brown/yellow was observed alongside the precipitation of a solid. Solvents were removed *in vacuo* and the remaining dark brown solid was washed with hexane (1 x 1 mL), dried *in vacuo* and redissolved in toluene (1 mL) to give a dark brown solution. The solution was filtered and layered with hexane. A combination of colourless and dark crystals were formed and characterized by singe crystal X-ray diffraction as [Ni(IMes)$_2$][Bcat$_2$] (**6**) and [Ni$_2$(IMes)$_2$][Bcat$_2$] (**7**) respectively.

X-Ray Crystallography

Single crystal X-ray diffraction data for [Ni(IMes)$_2$(Bcat)Cl] (**2**) was collected on a Bruker APEX-2 CCD diffractometer using Mo-Kα (λ = 0.71073 Å) radiation. The crystal was kept at 100 K during data collection. Using Olex2[6], the structure was solved with the SHELXS[7] structure solution program using Direct Methods and refined with the SHELXL[8] refinement package using Least Squares minimisation. Non-hydrogen atoms were refined anisotropically and hydrogen atoms were placed in calculated positions, refined using a riding model. The crystal structure image was made using Mercury.

Single crystal X-ray diffraction data for **2, 3** and **5-7** were collected on a RIGAKU Oxford Supernova Dual EosS2 diffractometer using Cu-Kα (λ = 1.54184 Å) radiation. The crystals were kept at 150 K during data collection. Using Olex2[6], the structures were solved with the SHELXT[9] structure solution program using Intrinsic Phasing and refined with the SHELXL[8] refinement package using Least Squares minimisation. Non-hydrogen atoms were refined anisotropically and hydrogen atoms were placed in calculated positions, refined using a riding model. Crystal structure images were made using Mercury.

Supplementary crystallographic data for compounds **2, 3** and **5-7** can be obtained from the Cambridge Crystallographic Data Centre as CCDC 2304318, 2304313, 2304314, 2304315, 2304316, 2304317.

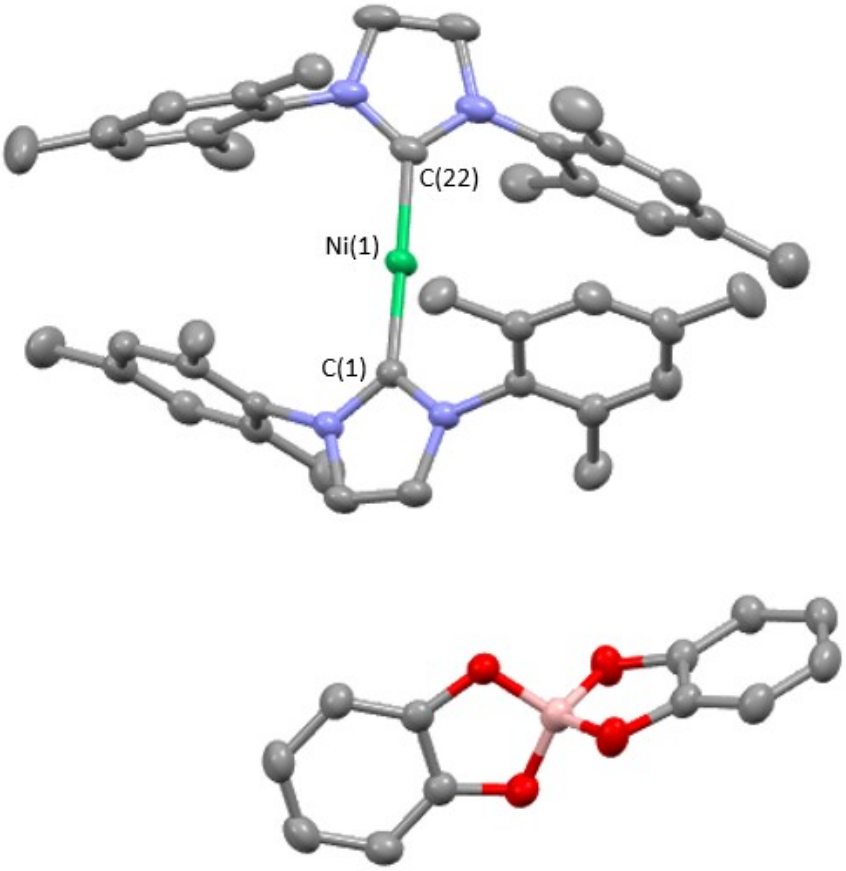


Figure S17. Molecular structure of **6** as determined by single crystal X-ray diffraction. Thermal ellipsoids set at the 50 % probability level and hydrogen atoms omitted for clarity.

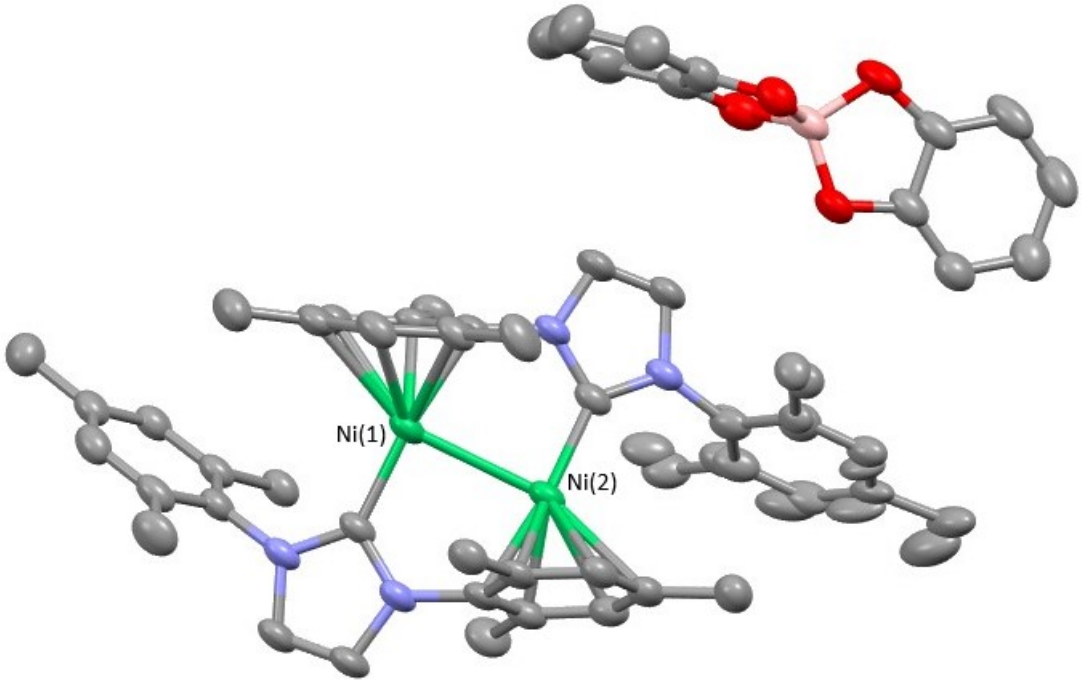


Figure S18. Molecular structure of **7** as determined by single crystal X-ray diffraction. Thermal ellipsoids set at the 50 % probability level and hydrogen atoms omitted for clarity.

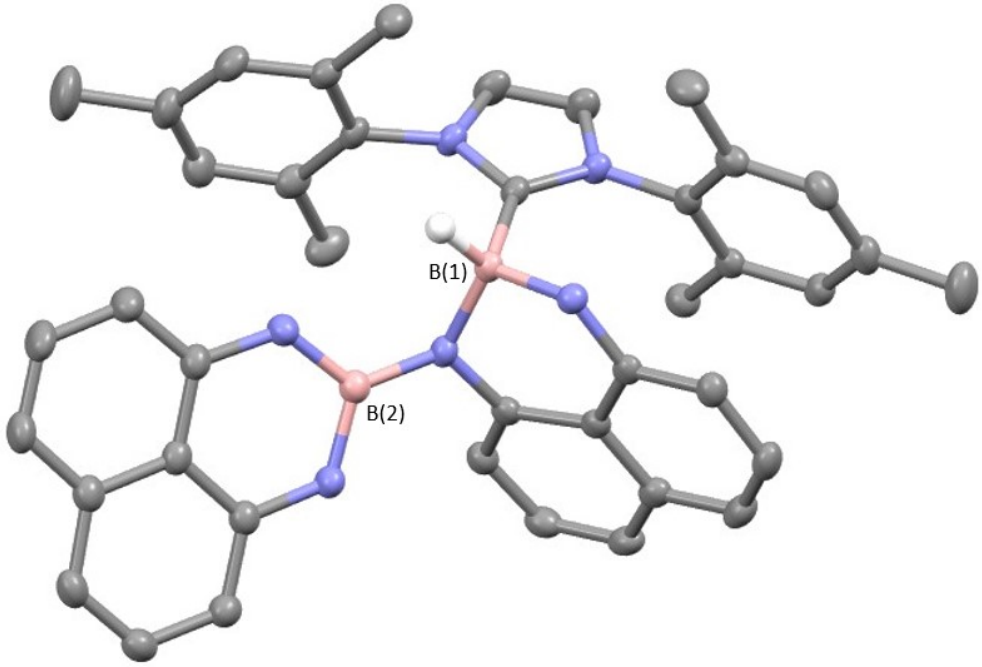


Figure S19. Molecular structure of the product of dehydrocoupling as determined by single crystal X-ray diffraction. Thermal ellipsoids set at the 50 % probability level and hydrogen atoms omitted for clarity.

Crystallographic Data

Compound	$Ni(IMes)_2(Bcat)Cl$	$Ni(IMes)_2(Bdan)Cl$	$Ni(IMes)_2(Bdan)Me$
Empirical formula	$C_{48}H_{52}BClN_4NiO_2$	$C_{55.5}H_{60}BClN_6Ni$	$C_{57}H_{69}BN_6NiO$
Formula weight	821.90	916.06	923.70
Temperature/K	100.0	150.00(10)	150.00(10)
Crystal system	monoclinic	monoclinic	triclinic
Space group	$P2_1/n$	$P2_1/c$	P-1
a/Å	10.482(4)	17.9362(6)	11.4827(3)
b/Å	13.929(5)	11.3297(4)	15.0976(4)
c/Å	33.577(13)	24.0854(9)	15.7441(5)
α/°	90	90	85.618(2)
β/°	96.737(7)	96.570(3)	84.570(2)
γ/°	90	90	75.422(2)
Volume/Å^3	4868(3)	4862.3(3)	2625.77(13)
Z	4	4	2
ρ_{calc}g/cm^3	1.121	1.251	1.168
μ/mm^{-1}	0.492	1.407	0.862
F(000)	1736.0	1940.0	988.0
Crystal size/mm^3	0.34 × 0.22 × 0.2	0.104 × 0.083 × 0.071	0.122 × 0.101 × 0.098
Radiation	Mo Kα (λ = 0.71073)	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	2.442 to 55.018	8.418 to 146.734	7.98 to 146.632
Index ranges	-13 ≤ h ≤ 13, -18 ≤ k ≤ 18, -43 ≤ l ≤ 43	-22 ≤ h ≤ 22, -14 ≤ k ≤ 14, -29 ≤ l ≤ 29	-14 ≤ h ≤ 13, -18 ≤ k ≤ 17, -19 ≤ l ≤ 19
Reflections collected	171407	15659	33095
Independent reflections	11177 [R_{int} = 0.1452, R_{sigma} = 0.0621]	15659 [R_{int} = ?, R_{sigma} = 0.0818]	10494 [R_{int} = 0.0344, R_{sigma} = 0.0354]
Data/restraints/parameters	11177/0/526	15659/25/600	10494/3/574
Goodness-of-fit on F^2	1.027	0.827	1.048
Final R indexes [I>=2σ (I)]	R_1 = 0.0522, wR_2 = 0.1122	R_1 = 0.0457, wR_2 = 0.1028	R_1 = 0.0380, wR_2 = 0.1009
Final R indexes [all data]	R_1 = 0.0886, wR_2 = 0.1268	R_1 = 0.0833, wR_2 = 0.1114	R_1 = 0.0465, wR_2 = 0.1058
Largest diff. peak/hole / e Å^{-3}	0.31/-0.71	0.40/-0.27	0.26/-0.29

Compound	$[Ni(IMes)_2][Bcat_2]$	$[Ni_2(IMes)_2][Bcat_2]$	IMes.HBdanBdan
Empirical formula	$C_{54}H_{56}BN_4NiO_4$	$C_{55.2}H_{57}BN_4Ni_2O_4F_{0.2}$	$C_{41}H_{40}B_2N_6$
Formula weight	894.54	972.47	638.41
Temperature/K	150.00(10)	150.01(10)	150.00(10)
Crystal system	monoclinic	triclinic	monoclinic
Space group	$P2_1/c$	P-1	$P2_1/c$
a/Å	12.2169(2)	12.0673(3)	12.53560(10)
b/Å	15.9479(2)	13.4580(5)	7.89280(10)
c/Å	24.7366(4)	15.2235(5)	33.1689(3)
α/°	90	91.823(3)	90
β/°	98.3640(10)	99.146(3)	92.7810(10)
γ/°	90	97.973(3)	90
Volume/Å^3	4768.27(13)	2413.62(14)	3277.90(6)
Z	4	2	4
ρ_{calc}g/cm^3	1.246	1.338	1.294
μ/mm^{-1}	0.973	1.373	0.590
F(000)	1892.0	1022.0	1352.0
Crystal size/mm^3	0.094 × 0.074 × 0.047	0.097 × 0.061 × 0.037	0.222 × 0.099 × 0.08
Radiation	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	6.616 to 146.61	7.5 to 146.442	7.06 to 146.58
Index ranges	-14 ≤ h ≤ 15, -14 ≤ k ≤ 19, -29 ≤ l ≤ 30	-10 ≤ h ≤ 14, -16 ≤ k ≤ 16, -18 ≤ l ≤ 17	-15 ≤ h ≤ 14, -9 ≤ k ≤ 6, -41 ≤ l ≤ 39
Reflections collected	39214	27223	41247
Independent reflections	9486 [R_{int} = 0.0409, R_{sigma} = 0.0355]	9612 [R_{int} = 0.0368, R_{sigma} = 0.0392]	6578 [R_{int} = 0.0244, R_{sigma} = 0.0160]
Data/restraints/parameters	9486/0/589	9612/286/652	6578/3/464
Goodness-of-fit on F^2	1.085	1.015	1.021
Final R indexes [I>=2σ (I)]	R_1 = 0.0454, wR_2 = 0.1094	R_1 = 0.0426, wR_2 = 0.1024	R_1 = 0.0422, wR_2 = 0.1165
Final R indexes [all data]	R_1 = 0.0596, wR_2 = 0.1166	R_1 = 0.0570, wR_2 = 0.1108	R_1 = 0.0461, wR_2 = 0.1201
Largest diff. peak/hole / e Å^{-3}	0.43/-0.44	0.36/-0.50	0.26/-0.25

Computational

Computational Details

All geometry DFT optimisations were performed using Gaussian 09 (Revision D.01)[10] and the BP86 functional.[11, 12] Ni and Cl centres were described with the Stuttgart RECPs and the corresponding basis sets[13] and d-orbital polarisation was added for Cl (ζ = 0.640).[14] 6-31G(d,p) basis sets were used to describe all other centres.[15] The polarizable continuum model (PCM) was included in the optimisation protocol to model the effect of the toluene solvent and its corresponding dielectric constant (ε = 2.374).[16] Analytical frequency calculations were carried out to confirm minima as displaying no imaginary frequencies while transition states all present one negative frequency. The latter were validated by running IRCs and subsequent optimizations, connecting them to adjacent minima. Final free energies were obtained after corrections including the triple-ζ basis set Def2-TZVP[17] and dispersion using the D3BJ method.[18]

The structure of [Ni(IMes)$_2$] (**1**) was optimised without any symmetry constraints and converged on a structure with effective D_{2d} symmetry, similar to that reported by Radius and co-workers.[19] The computed structure with the methodology used here displays one imaginary mode at -9.8 cm^{-1} which despite many attempts could not be removed.

Computed Reaction Profiles and Alternative Mechanisms with XBdan (X = Cl, H)

B–Cl Activation by Nucleophilic Displacement Involving Triplet States

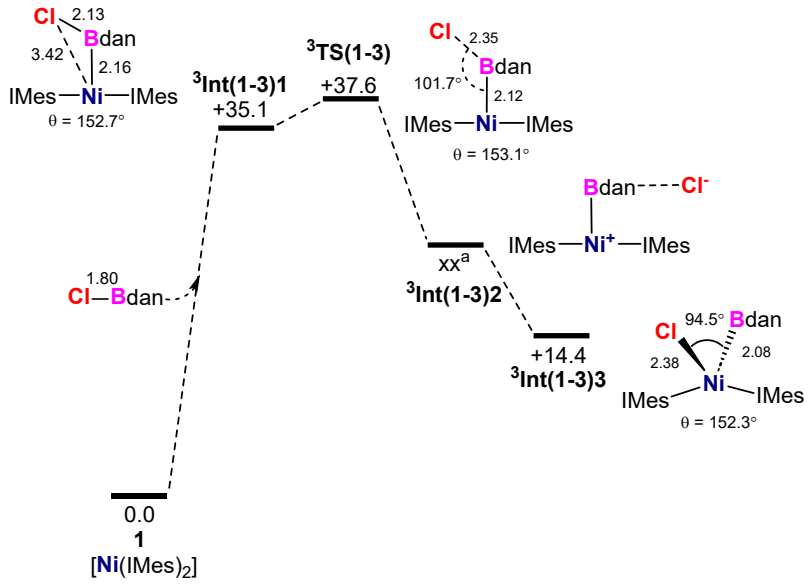


Figure S20: Computed free energy reaction profile (kcal mol^{-1}) for B–Cl activation of ClBdan at Ni(IMes)$_2$ involving triplet states only. [a]SCF convergence failure.

B–Cl Activation by Nucleophilic Displacement Involving Singlet States Optimised in Gas Phase

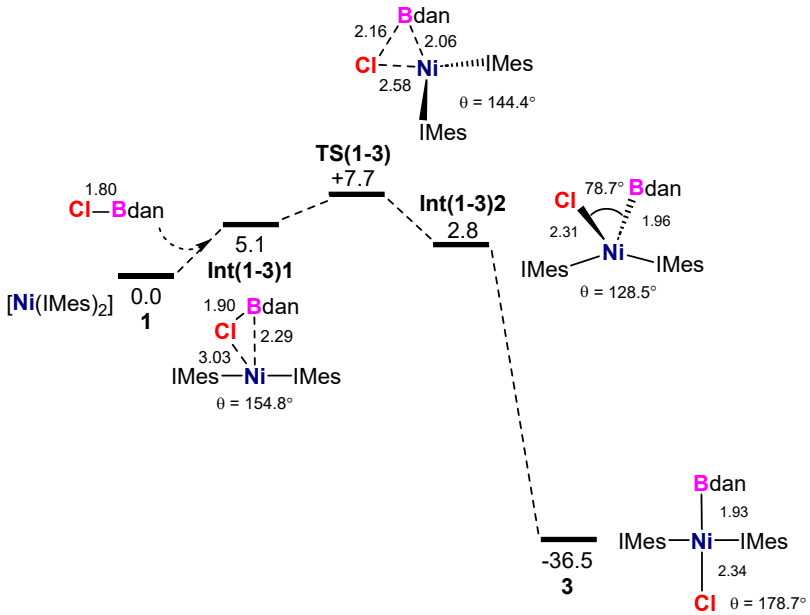


Figure S21: Computed free energy reaction profile (kcal mol^{-1}) for B–Cl activation of ClBdan at Ni(IMes)$_2$ involving singlet states only, optimised in gas phase without solvation energy correction.

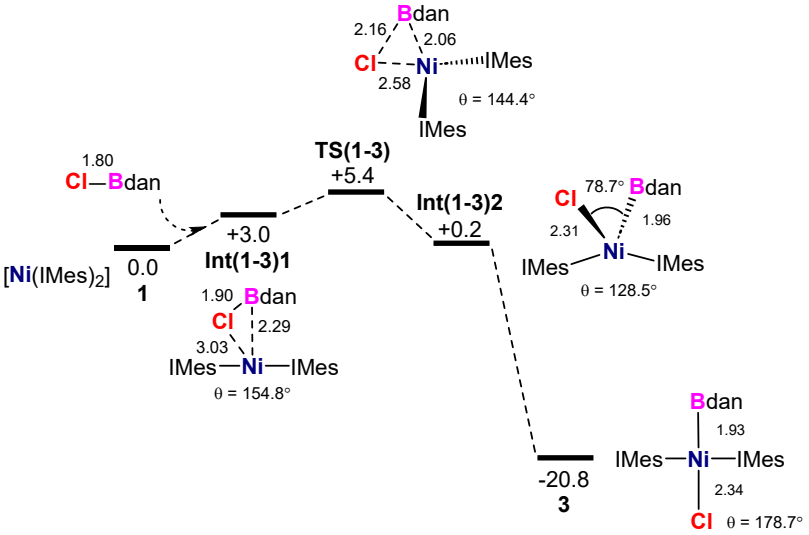


Figure S22: Computed free energy reaction profile (kcal mol^{-1}) for B–Cl activation of ClBdan at Ni(IMes)$_2$ involving singlet states only, optimised in gas phase including further solvation energy correction.

B–H Activation Involving Singlet States

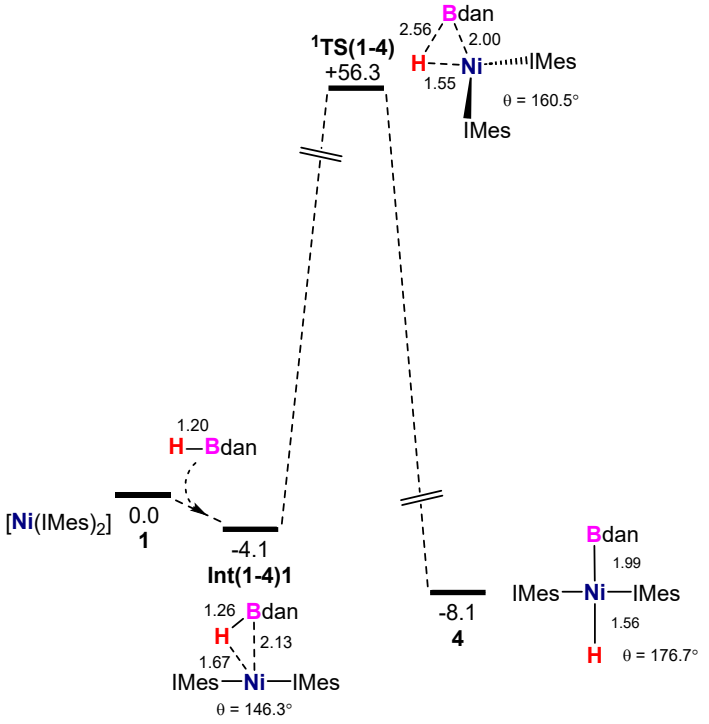


Figure S23: Computed free energy reaction profile (kcal mol^{-1}) for B–H activation of HBdan at Ni(IMes)$_2$ involving singlet states only.

B–H Activation Involving Triplet States

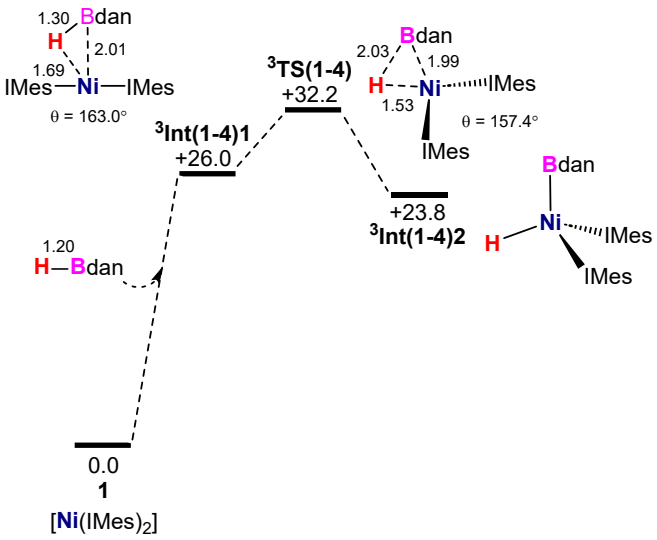


Figure S24: Computed free energy reaction profile (kcal mol^{-1}) for B–H activation of HBdan at Ni(IMes)$_2$ involving triplet states only.

HBdan / IMes Coupling at Int(1-4)1 Followed by Dehydrocoupling

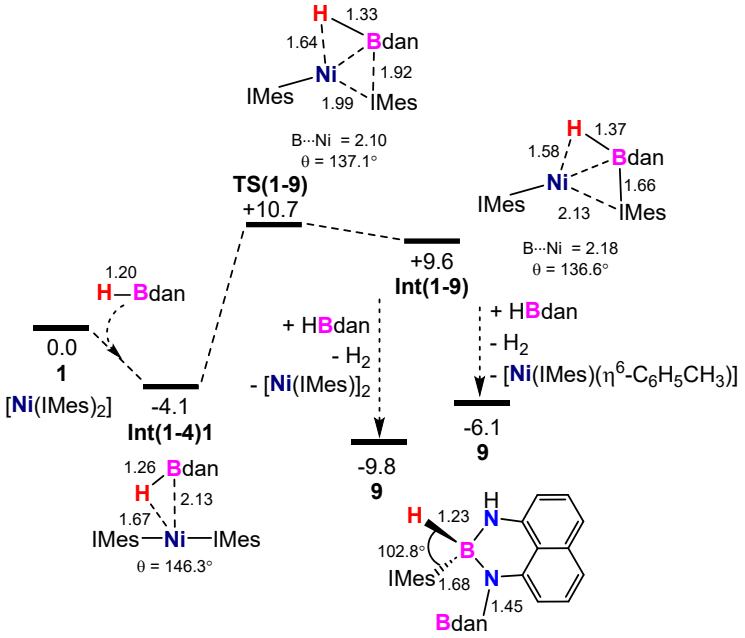


Figure S25: Computed free energy reaction profile (kcal mol^{-1}) for HBdan coupling with IMes at **Int(1-4)1**. The thermodynamics of dehydrocoupling to give **9** is indicated with the formation of either dimeric [Ni(IMes)]$_2$ or monomeric [Ni(IMes)(η^6-C$_6$H$_5$CH$_3$)].

Alternative Radical Processes

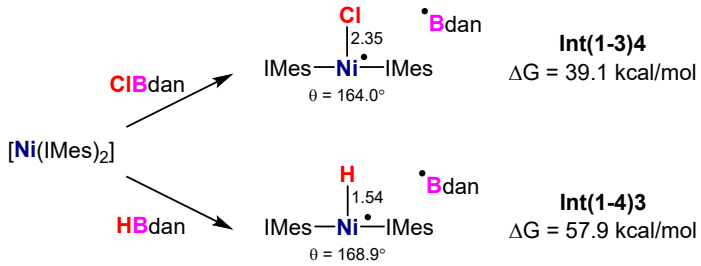


Figure S26: Computed free energy (kcal mol^{-1}) for B–X activation of XBdan (X = Cl, H) at Ni(IMes)$_2$ by X atom transfer and formation of a Bdan radical.

Alternative N–H Activation

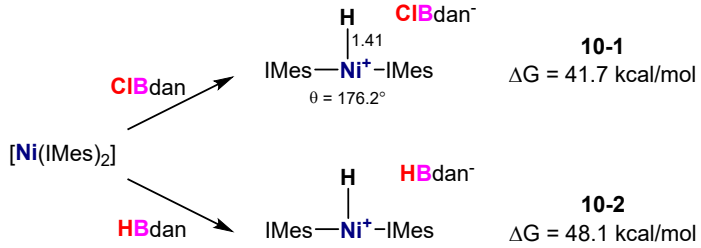


Figure S27: Computed free energy (kcal mol^{-1}) for N–H activation of XBdan (X = Cl, H) at Ni(IMes)$_2$ by proton transfer. This was modelled as separate ions as all attempts to locate the ion pair led to deprotonation of the Ni–hydride, suggesting, along with the unfavourable thermodynamics, that this process is not accessible.

Computed Reaction Profiles with XBcat (X = Cl, H)

B–Cl Activation by Nucleophilic Displacement Involving Singlet States

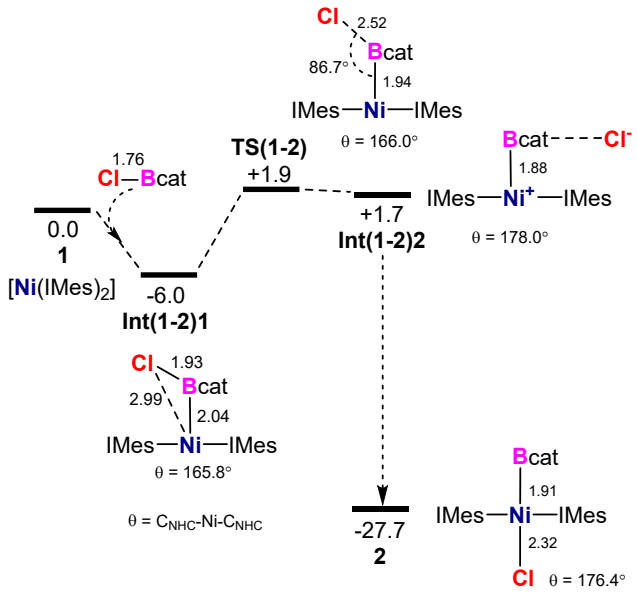


Figure S28: Computed free energy reaction profile (kcal mol^{-1}) for B–Cl activation of ClBcat at Ni(IMes)$_2$ involving singlet states only.

B–H Activation by Oxidative Addition Involving Singlet States

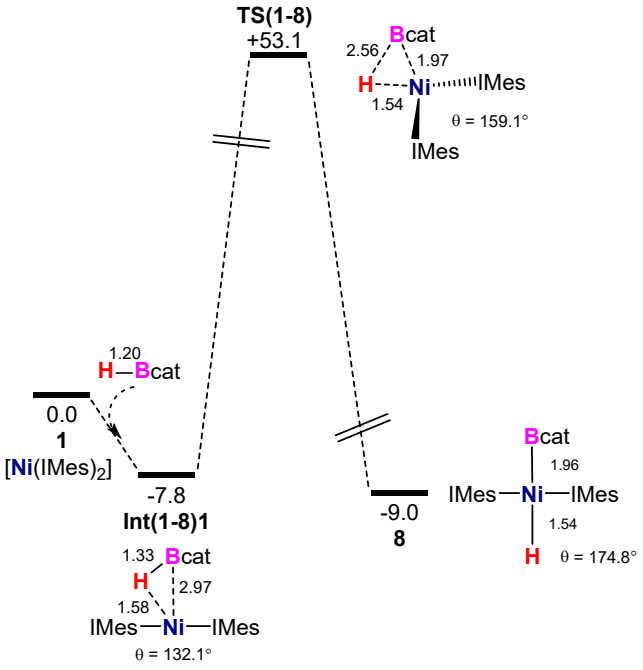


Figure S29: Computed free energy reaction profile (kcal mol^{-1}) for B–H activation of HBcat at Ni(IMes)$_2$ involving singlet states only.

B–H Activation by Oxidative Addition Involving Triplet States

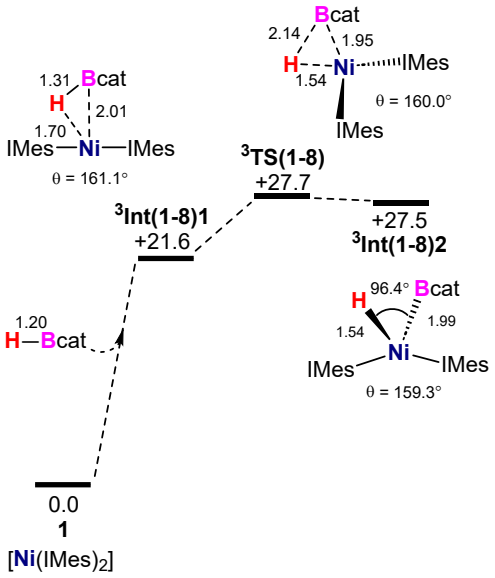


Figure S30: Computed free energy reaction profiles (kcal mol^{-1}) for B–H activation of HBcat at Ni(IMes)$_2$ involving triplet states only.

HBcat / IMes Coupling at Int(1-5)1

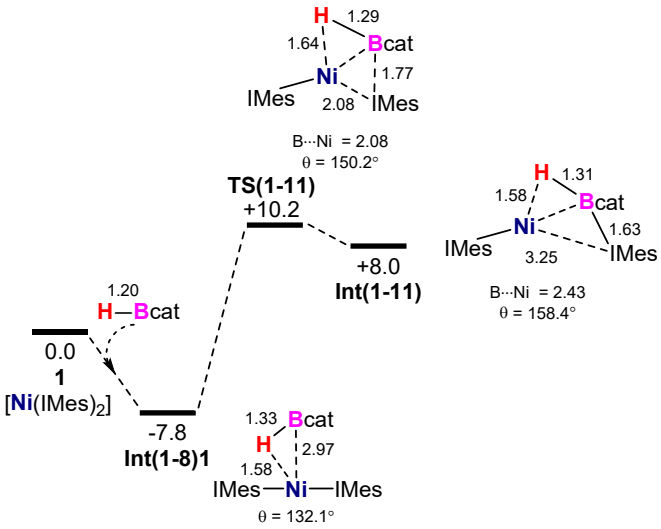


Figure S31: Computed free energy reaction profile (kcal mol^{-1}) for HBcat/IMes coupling at **Int(1-8)1**. The energetics of the subsequent dehydrocoupling were not considered.

Alternative Radical Processes

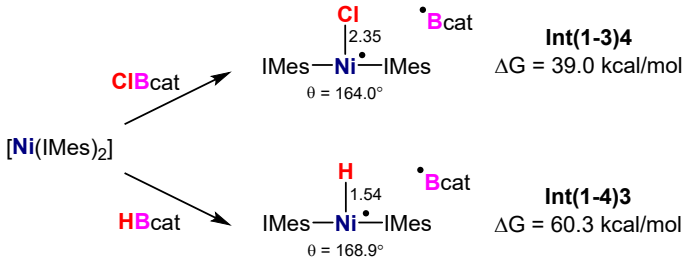
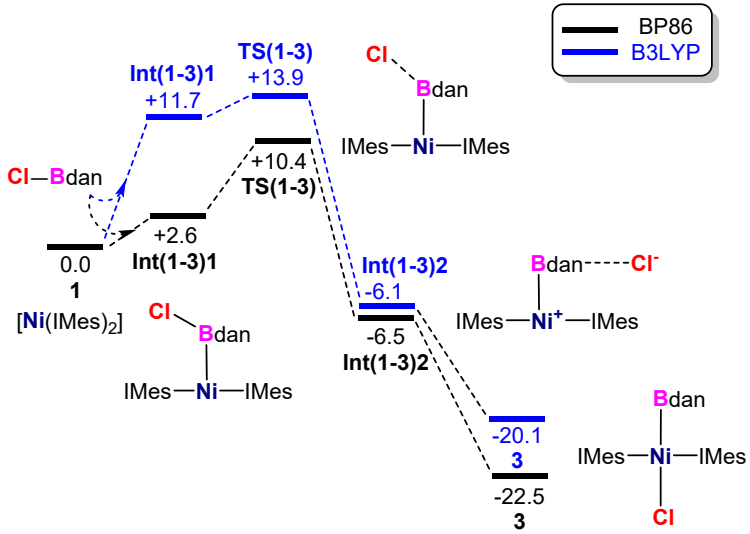


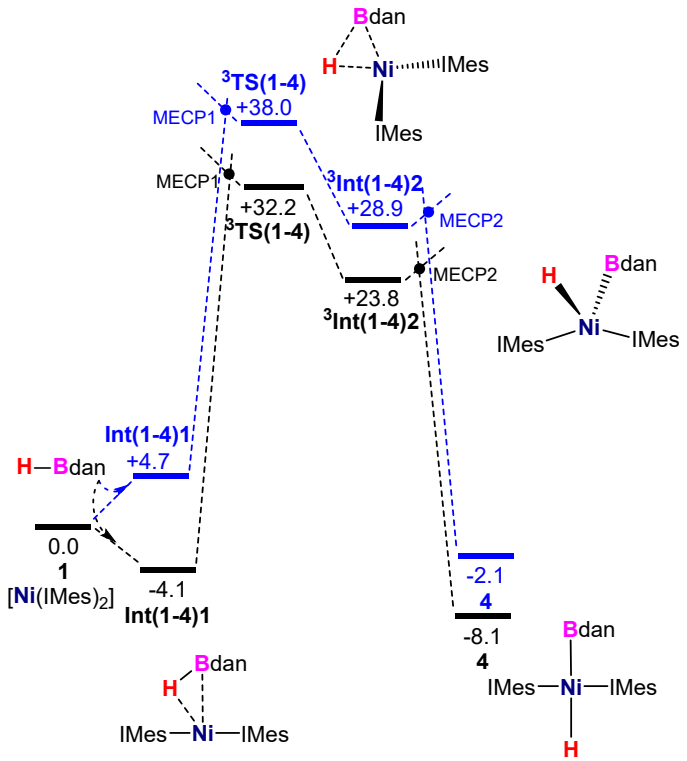
Figure S32: Computed free energy (kcal mol^{-1}) for B–X activation of XBcat (X = Cl, H) at $Ni(IMes)_2$ by X atom transfer and formation of a Bcat radical.

Functional Testing



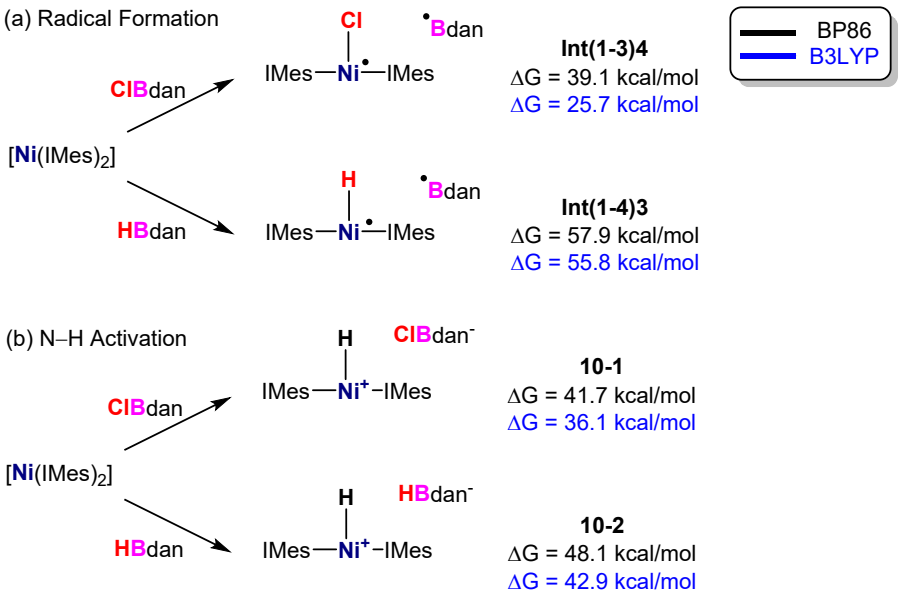
	BP86	BLYP	B3LYP	B3PW91	PBE	PBE0	B97D3	B97D	M06	wB97xD	TPSS
Int(1-3)1	2.6	8.5	11.7	6.9	10.6	12.7	10.4	10.2	20.2	14.3	8.2
TS(1-3)	10.4	13.9	13.9	11.3	19.2	16.7	16.6	15.8	27.0	15.3	15.5
Int(1-3)2	-6.5	-4.0	-6.1	-8.2	1.6	-3.6	-1.9	-2.3	9.1	-6.6	-2.3
3	-22.5	-16.7	-20.1	-24.4	-13.9	-20.3	-13.4	-11.2	-6.5	-20.9	-18.7

Figure S33: Computed free energy reaction profiles (kcal mol^{-1}) for B–Cl activation to assess functional dependence of the proposed reactivity. The profile highlights the GGA functional BP86 and hybrid B3LYP, showing in both cases, results in alignment with experiment.



	BP86	BLYP	B3LYP	B3PW91	PBE	PBE0	B97D3	B97D	M06	wB97xD	TPSS
Int(1-4)1	-4.1	2.7	4.7	-0.7	0.9	2.7	3.2	2.6	12.4	3.5	0.0
^{3}Int(1-4)1	26.0	33.6	27.6	20.8	30.4	21.0	34.8	33.0	34.7	26.6	28.0
^{3}TS(1-4)	32.2	40.7	38.0	30.9	36.8	31.7	41.5	40.6	47.0	36.1	34.3
^{3}Int(1-4)2	23.8	31.8	28.9	22.3	29.6	23.7	33.0	32.6	39.3	97.3	26.3
4	-8.1	0.3	-2.1	-8.7	-1.5	-5.6	1.9	1.7	9.9	-5.8	-2.8

Figure S34: Free energies of selected stationary points (kcal mol^{-1}) for B–H activation to assess functional dependence of the proposed reactivity. The profile highlights the GGA functional BP86 and hybrid B3LYP, showing in both cases, results in alignment with experiment.



	BP86	BLYP	B3LYP	B3PW91	PBE	PBE0	B97D3	B97D	M06	wB97xD	TPSS
Int(1-3)4	39.1	38.4	25.7	25.5	42.2	23.4	41.9	43.4	34.3	23.7	35.1
Int(1-4)3	57.9	60.5	55.8	53.0	59.2	51.7	62.2	63.4	63.2	54.8	57.2
10-1	41.7	41.3	36.1	35.9	42.5	35.1	42.0	42.3	46.5	35.1	38.4
10-2	48.1	47.8	42.9	42.6	48.8	41.7	48.5	48.8	53.3	42.1	45.1

Figure S35: Computed free energies (kcal mol^{-1}) for (a) X atom transfer and formation of a Bdan radical and (b) N–H activation to assess functional dependence of the proposed reactivity. The profile highlights the GGA functional BP86 and hybrid B3LYP, showing in both cases consistent results in that these processes are highly disfavoured.

Computed Structures (Å) and Energies (atomic units)

1

SCF = -2019.48879919
H(0 K)= -2018.716137
H(298 K)= -2018.663878
G(298 K)= -2018.808324
SCF(D3BJ) = -2019.72364323
SCF(BS2) = -3357.65448343
SCF(BS2+D3BJ) = -3357.88932745
Low Freq. = -9.7745cm-1, 11.3746cm-1

C	0.61006	-0.47449	-4.04726
C	-0.37071	0.47634	-4.07270
C	0.05864	-0.00253	-1.84280
N	0.86156	-0.75603	-2.69878
N	-0.69590	0.75386	-2.73933
Ni	0.00119	-0.00596	0.00048
C	-0.05545	-0.00847	1.84395
N	-0.83328	-0.78833	2.69924
N	0.67503	0.77068	2.74096
C	-0.59009	-0.50050	4.04799
C	0.36013	0.48084	4.07413
H	-1.10783	-1.01765	4.85197
H	0.83889	0.99219	4.90554
H	1.14461	-0.97372	-4.85158
H	-0.86403	0.97446	-4.90363
C	1.64404	1.76416	2.35166
C	2.99208	1.37670	2.17510
C	1.22920	3.10796	2.20651
C	3.92794	2.37454	1.84652
C	2.20379	4.06790	1.87782
C	3.55735	3.72458	1.69803
H	4.97645	2.08578	1.70209
H	1.89325	5.11321	1.75696
C	-1.79005	-1.77207	2.25798
C	-3.13993	-1.38716	2.08794
C	-1.36427	-3.10516	2.05704
C	-4.06624	-2.37631	1.70966
C	-2.32959	-4.05658	1.67936
C	-3.68457	-3.71587	1.50538
H	-5.11580	-2.08901	1.57004
H	-2.01054	-5.09366	1.51695
C	1.84279	-1.71549	-2.25788
C	3.18255	-1.29757	-2.08678
C	1.44965	-3.05877	-2.05777
C	4.13229	-2.26348	-1.70649
C	2.43744	-3.98596	-1.67817
C	3.78322	-3.61191	-1.50195
H	5.17420	-1.95006	-1.56547
H	2.14432	-5.03065	-1.51601
C	-1.69418	1.71806	-2.35050
C	-3.03448	1.29571	-2.19545
C	-1.31453	3.06991	-2.18620
C	-3.99900	2.26681	-1.86990
C	-2.31682	4.00216	-1.86110
C	-3.66370	3.62406	-1.70341
H	-5.04170	1.95051	-1.74165
H	-2.03415	5.05355	-1.72584
C	-0.22384	3.49236	2.36696
H	-0.84541	2.96497	1.62105
H	-0.61438	3.21516	3.36189
H	-0.36048	4.57729	2.23376
C	3.40465	-0.07134	2.30365
H	3.12689	-0.49017	3.28680
H	2.89309	-0.68410	1.53888
H	4.49294	-0.18379	2.17519
C	4.59225	4.78461	1.38259
H	5.00731	5.22749	2.30727
H	5.43936	4.36620	0.81412
H	4.15914	5.61041	0.79388
C	0.09002	-3.48696	2.20994
H	0.48739	-3.19963	3.19902
H	0.22682	-4.57281	2.08432
H	0.70541	-2.96417	1.45473
C	-3.56562	0.05101	2.27552
H	-3.31461	0.42508	3.28357
H	-3.04326	0.70400	1.55323
H	-4.65152	0.16228	2.12736
C	-4.70982	-4.76904	1.13963
H	-5.13725	-5.24266	2.04321
H	-5.55000	-4.33587	0.57190
H	-4.26422	-5.57394	0.53172
C	-3.40929	-0.16100	-2.34189
H	-3.11746	-0.56198	-3.32843
H	-2.88579	-0.76903	-1.58163
H	-4.49489	-0.30227	-2.21934
C	0.13077	3.49049	-2.32233
H	0.54604	3.21821	-3.30850
H	0.23803	4.57905	-2.19168
H	0.75131	2.98149	-1.56259
C	-4.72887	4.65510	-1.39261
H	-5.16729	5.07040	-2.31934
H	-5.55682	4.21851	-0.80961
H	-4.31647	5.50268	-0.82042
C	3.57353	0.15017	-2.27649
H	3.32303	0.51360	-3.28862
H	3.02834	0.79319	-1.56231
H	4.65490	0.28897	-2.11906
C	0.00556	-3.47575	-2.21455
H	-0.39484	-3.19992	-3.20568
H	-0.10612	-4.56424	-2.08690
H	-0.62459	-2.96585	-1.46276
C	4.83324	-4.63950	-1.13371
H	5.28196	-5.09468	-2.03645
H	5.65613	-4.18814	-0.55488
H	4.40364	-5.46043	-0.53584

ClBdan

SCF = -535.423336911
H(0 K)= -535.261163
H(298 K)= -535.249656
G(298 K)= -535.297431
SCF(D3BJ) = -535.472266590
SCF(BS2) = -980.837452225
SCF(BS2+D3BJ) = -980.886381904

Low Freq. = 83.1277cm-1,
130.2839cm-1

C	2.14681	2.44498	-0.00002
H	2.68382	3.39943	-0.00003
C	2.85552	1.25163	0.00000
H	3.95048	1.25255	0.00005
C	2.16849	0.00000	0.00001
C	2.14682	-2.44497	0.00005
H	2.68383	-3.39942	0.00009
C	2.85553	-1.25162	0.00002
H	3.95049	-1.25254	-0.00001
H	0.18531	-3.40694	0.00008
C	0.73061	-2.45676	0.00004
C	0.02358	-1.25247	-0.00004
C	0.72720	0.00000	-0.00001
C	0.02357	1.25246	-0.00002
C	0.73060	2.45676	-0.00006
H	0.18530	3.40694	-0.00009
N	-1.38276	-1.21941	-0.00009
H	-1.85429	-2.12234	-0.00053
B	-2.11153	-0.00001	0.00002
N	-1.38276	1.21940	0.00003
H	-1.85430	2.12233	0.00060
Cl	-3.90981	0.00000	0.00002

HBdan

SCF = -520.945949834
H(0 K)= -520.775886
H(298 K)= -520.765743
G(298 K)= -520.809752
SCF(D3BJ) = -520.991240597
SCF(BS2) = -521.129367594
SCF(BS2+D3BJ)= -521.174658357
Low Freq. = 134.4623cm-1,
155.7653cm-1

C	-2.44545	-1.42937	-0.00004
H	-3.40010	-1.96660	-0.00007
C	-1.25228	-2.13950	-0.00001
H	-1.25411	-3.23461	0.00001
C	-0.00021	-1.45299	0.00000
C	2.44504	-1.43007	0.00004
H	3.39953	-1.96758	0.00007
C	1.25167	-2.13985	0.00002
H	1.25318	-3.23497	0.00000
H	3.40670	0.53133	0.00004
C	2.45660	-0.01449	0.00003
C	1.25171	0.69504	-0.00002
C	-0.00001	-0.01137	-0.00001
C	-1.25152	0.69540	0.00002
C	-2.45661	-0.01378	-0.00003
H	-3.40656	0.53230	-0.00004
N	1.21339	2.09737	-0.00009
H	2.11998	2.56128	-0.00024
B	0.00042	2.84955	-0.00002
N	-1.21277	2.09772	0.00009
H	-2.11922	2.56192	0.00030
H	0.00057	4.04946	0.00004

ClBcat

SCF = -421.501046967
H(0 K)= -421.409090
H(298 K)= -421.400705
G(298 K)= -421.441801
SCF(DJD3) = -421.526267978
SCF(BS2) = -866.888501510
SCF(BS2+DJD3) = -866.913722525
Low Freq. = 97.6555cm-1,
192.4032cm-1

C	-1.75597	1.44424	0.00004
C	-2.95700	0.70410	-0.00001
H	-3.90995	1.24038	-0.00003
C	-2.95679	-0.70448	0.00000
H	-3.90959	-1.24105	0.00003
C	-1.75562	-1.44435	-0.00004
H	-1.74423	-2.53658	-0.00003
H	-1.74465	2.53644	0.00003
C	-0.57835	0.70209	0.00002
C	-0.57800	-0.70208	-0.00004
O	0.73923	-1.16228	0.00007
O	0.73897	1.16275	-0.00003
B	1.50313	0.00048	0.00002
Cl	3.26221	-0.00014	-0.00001

HBcat

SCF = -407.027276190
H(0 K)= -406.927685
H(298 K)= -406.920539
G(298 K)= -406.958003
SCF(DJD3) = -407.049749760
SCF(BS2) = -407.183172221
SCF(BS2+DJD3)= -407.205645790
Low Freq. = 216.8229cm-1,
235.6984cm-1

C	0.90629	-1.44339	0.00000
C	2.10771	-0.70453	0.00000
H	3.06136	-1.24110	0.00000
C	2.10771	0.70453	0.00000
H	3.06136	1.24110	0.00000
C	0.90629	1.44339	0.00000
H	0.89507	2.53634	0.00000
H	0.89508	-2.53634	0.00000
C	-0.27338	-0.70212	0.00000
C	-0.27338	0.70212	0.00000
O	-1.58805	1.15795	0.00000
O	-1.58805	-1.15795	0.00000
B	-2.36671	-0.00001	0.00000
H	-3.55786	0.00002	0.00001

Int(1-3)1

SCF = -2554.89018403
H(0 K)= -2553.953330
H(298 K)= -2553.889087
G(298 K)= -2554.054207
SCF(D3BJ) = -2555.23175471
SCF(BS2) = -4338.45966991

SCF(BS2+D3BJ) = -4338.80124054
Low Freq. = 13.6411cm-1, 18.6588cm-1

C	-5.72454	2.18984	0.56073
C	-4.57915	3.02106	0.37259
C	-3.35841	2.42160	-0.10603
C	-3.32656	1.02282	-0.43487
C	-4.47451	0.23983	-0.22647
C	-5.65778	0.83165	0.27107
C	-2.18358	3.23075	-0.28618
C	-2.26396	4.61657	-0.06201
C	-3.46899	5.19629	0.39519
C	-4.60266	4.42568	0.62786
N	-1.00907	2.61496	-0.69329
B	-0.89160	1.20900	-1.09331
N	-2.16066	0.48760	-0.97952
Ni	0.47486	-0.22254	-0.12534
C	0.61434	-1.74452	-1.36482
N	-0.29691	-2.56343	-2.04005
C	0.33330	-3.51452	-2.85053
C	1.67223	-3.32806	-2.70426
N	1.83103	-2.26526	-1.81050
C	-1.73567	-2.63616	-1.91248
C	-2.54346	-2.25950	-3.01719
C	-3.92749	-2.49940	-2.92863
C	-4.51295	-3.11118	-1.80429
C	-3.67353	-3.48471	-0.73756
C	-2.28275	-3.27093	-0.77086
C	3.16258	-1.93559	-1.35459
C	3.99665	-1.13526	-2.16728
C	5.33000	-0.94962	-1.75445
C	5.84103	-1.53837	-0.58312
C	4.98820	-2.36629	0.17217
C	3.65319	-2.59822	-0.20496
C	3.48392	-0.51199	-3.44501
C	7.26866	-1.28855	-0.14516
C	2.78830	-3.58027	0.55215
C	-1.95323	-1.64085	-4.26464
C	-6.00798	-3.33835	-1.73943
C	-1.39847	-3.74603	0.35614
C	0.91044	0.76624	1.42497
N	0.87818	0.19230	2.70360
C	1.50067	0.98927	3.66851
C	1.93909	2.10477	3.02788
N	1.56867	1.98149	1.68357
C	0.27219	-1.05955	3.08919
C	-1.13835	-1.14421	3.18329
C	-1.69372	-2.33426	3.68621
C	-0.89610	-3.41738	4.10353
C	0.50128	-3.28153	4.02245
C	1.11111	-2.10908	3.53540
C	1.80024	3.09477	0.79338
C	1.18355	4.33751	1.09326
C	1.47077	5.43558	0.25867
C	2.33722	5.33417	-0.84562
C	2.94527	4.09046	-1.09293
C	2.70712	2.96398	-0.28318
C	0.23164	4.51276	2.25841
C	2.59102	6.52086	-1.75041
C	3.42116	1.66662	-0.54427
C	-2.01708	0.01828	2.79293
C	-1.52691	-4.69437	4.61763
C	2.61901	-1.97361	3.54238
Cl	0.06414	1.10804	-2.78086
H	-0.21910	3.24135	-0.84054
H	-2.22372	-0.49272	-1.25660
H	1.55818	0.69187	4.71177
H	2.48549	2.96937	3.39326
H	0.99478	6.39844	0.48112
H	3.64100	3.98938	-1.93458
H	4.01724	1.34911	0.32988
H	4.09629	1.75707	-1.40813
H	2.69703	0.85001	-0.73895
H	1.88108	6.53256	-2.59787
H	3.60682	6.49181	-2.17847
H	2.47099	7.47469	-1.21061
H	-0.45379	3.65579	2.35330
H	-0.37842	5.41832	2.12154
H	0.76715	4.61408	3.21924
H	-2.78504	-2.40707	3.76783
H	1.14241	-4.10379	4.36334
H	2.99277	-1.49319	2.62321
H	3.09587	-2.96148	3.64143
H	2.96752	-1.35712	4.39086
H	-2.46760	-4.49132	5.15627
H	-0.84979	-5.23456	5.29969
H	-1.77122	-5.38331	3.78768
H	-1.74688	0.92953	3.35576
H	-3.07757	-0.20492	2.98472
H	-1.89975	0.25892	1.72340
H	-0.23391	-4.23728	-3.43063
H	2.52426	-3.84879	-3.13304
H	5.98840	-0.32822	-2.37372
H	5.37916	-2.87127	1.06394
H	1.88730	-3.09815	0.96914
H	3.35175	-4.03902	1.37901
H	2.43772	-4.39113	-0.11142
H	7.92610	-1.08342	-1.00612
H	7.67993	-2.15131	0.40481
H	7.33109	-0.41373	0.52823
H	3.19876	-1.28178	-4.18442
H	4.25500	0.12715	-3.90374
H	2.58299	0.09776	-3.25916
H	-4.56331	-2.20352	-3.77140
H	-4.10778	-3.97580	0.14135
H	-0.64014	-4.46143	-0.00976
H	-1.99393	-4.24317	1.13673
H	-0.85258	-2.90528	0.81824
H	-6.40252	-3.70347	-2.70269
H	-6.53978	-2.39717	-1.50952
H	-6.27276	-4.06915	-0.95833
H	-1.25018	-0.82828	-4.01702
H	-2.75095	-1.23084	-4.90374
H	-1.39532	-2.38512	-4.86143
H	-1.37976	5.23731	-0.23975
H	-3.50177	6.27824	0.56966
H	-5.52900	4.88378	0.99107
H	-4.44260	-0.82798	-0.46231
H	-6.54118	0.19995	0.42225
H	-6.65202	2.64034	0.93080

TS(1-3)

SCF = -2554.88358879
H(0 K)= -2553.946214
H(298 K)= -2553.882520
G(298 K)= -2554.046707
SCF(D3BJ) = -2555.22421252
SCF(BS2) = -4338.44900677
SCF(BS2+D3BJ) = -4338.78963050
Low Freq. = -81.8875cm-1, 10.1166cm-1

C	-4.54498	4.45788	-0.44305
C	-3.13435	4.66521	-0.36287
C	-2.26512	3.51486	-0.35159
C	-2.82415	2.19798	-0.46419
C	-4.21493	2.03672	-0.53406
C	-5.06143	3.17051	-0.52142
C	-0.84365	3.69204	-0.24626
C	-0.31097	4.99101	-0.22753
C	-1.17047	6.11311	-0.25481
C	-2.55220	5.96700	-0.30414
N	-0.03540	2.56015	-0.14947
B	-0.51195	1.22105	-0.42034
N	-1.94981	1.10378	-0.49965
Ni	0.43300	-0.46966	0.03432
C	0.20656	-1.54980	-1.56757
N	-0.89729	-1.94646	-2.31098
C	-0.53551	-2.75163	-3.39411
C	0.81663	-2.90153	-3.34040
N	1.25481	-2.17984	-2.22855
C	-2.30271	-1.75770	-2.01921
C	-3.09050	-0.96241	-2.88999
C	-4.47789	-0.91413	-2.64914
C	-5.08790	-1.62956	-1.60152
C	-4.27098	-2.42591	-0.77816
C	-2.88081	-2.52192	-0.97609
C	2.63792	-2.27860	-1.81117
C	3.63730	-1.58834	-2.53803
C	4.97979	-1.81646	-2.17443
C	5.34409	-2.70547	-1.14793
C	4.31941	-3.39873	-0.47527
C	2.96340	-3.21510	-0.79898
C	3.29827	-0.66949	-3.68556
C	6.79613	-2.90816	-0.77007
C	1.89602	-4.04621	-0.12189
C	-2.48444	-0.19286	-4.03833
C	-6.57993	-1.53617	-1.36129
C	-2.04983	-3.45213	-0.12564
C	0.78842	0.14270	1.79607
N	0.23429	-0.44258	2.93346
C	0.79334	0.05732	4.11036
C	1.71812	0.98549	3.73884
N	1.70687	1.03809	2.34427
C	-0.75032	-1.50170	3.00745
C	-2.12521	-1.16738	3.01531
C	-3.04777	-2.20775	3.23127
C	-2.64196	-3.53647	3.45973
C	-1.26377	-3.81848	3.47578
C	-0.29697	-2.81715	3.26658
C	2.58567	1.95989	1.65812
C	2.38124	3.35045	1.84121
C	3.27897	4.23200	1.20921
C	4.35833	3.77306	0.43144
C	4.55076	2.38442	0.31934
C	3.68776	1.45691	0.93120
C	1.25114	3.89549	2.68813
C	5.27802	4.74484	-0.27521
C	3.96251	-0.02243	0.83954
C	-2.58901	0.25903	2.84452
C	-3.66265	-4.63371	3.67536
C	1.17715	-3.13924	3.38801
Cl	0.52601	1.38502	-2.88673
H	0.96296	2.74400	-0.23474
H	-2.38639	0.20107	-0.68542
H	0.47834	-0.29551	5.08857
H	2.38882	1.60459	4.32757
H	3.12562	5.31078	1.33246
H	5.40481	2.00422	-0.25334
H	3.86908	-0.51269	1.82417
H	4.97544	-0.20712	0.45224
H	3.25006	-0.52030	0.15810
H	4.91753	4.95033	-1.29965
H	6.30027	4.34146	-0.36459
H	5.33146	5.71080	0.25334
H	0.32825	3.31082	2.55101
H	1.03374	4.93877	2.41413
H	1.50300	3.87903	3.76415
H	-4.11650	-1.96305	3.24292
H	-0.92565	-4.84246	3.67556
H	1.78149	-2.61476	2.63042
H	1.34913	-4.22183	3.28283
H	1.57066	-2.83641	4.37580
H	-4.57201	-4.24838	4.16525
H	-3.25537	-5.44882	4.29576
H	-3.97673	-5.08237	2.71448
H	-2.12034	0.92483	3.59066
H	-3.68126	0.33149	2.96074
H	-2.31927	0.65012	1.84881
H	-1.27614	-3.14999	-4.08162
H	1.50480	-3.45747	-3.97113
H	5.76419	-1.28607	-2.72773
H	4.58037	-4.12310	0.30605
H	1.15817	-3.42238	0.41140
H	2.34745	-4.74122	0.60299
H	1.32852	-4.64230	-0.85898
H	7.46864	-2.67601	-1.61191
H	6.99001	-3.94547	-0.44967
H	7.08505	-2.25043	0.07066
H	2.94641	-1.24165	-4.56392
H	4.18704	-0.09771	-3.99699
H	2.48684	0.03566	-3.42080
H	-5.09739	-0.29610	-3.30934
H	-4.72706	-3.01521	0.02625
H	-1.42175	-4.11070	-0.75081
H	-2.69608	-4.08329	0.50260
H	-1.37140	-2.89153	0.54102
H	-7.13431	-1.41727	-2.30681
H	-6.82801	-0.66413	-0.72844
H	-6.96269	-2.43270	-0.84632
H	-1.56881	0.34472	-3.72702

H -3.20848 0.53651 -4.43424
H -2.20003 -0.86472 -4.86913
H 0.77544 5.12315 -0.19205
H -0.73015 7.11686 -0.23463
H -3.20925 6.84339 -0.31533
H -4.63372 1.02911 -0.61893
H -6.14590 3.02210 -0.58238
H -5.20891 5.32930 -0.44786

Int(1-3)2
SCF = -2554.91086863
H(0 K)= -2553.972563
H(298 K)= -2553.908327
G(298 K)= -2554.074019
SCF(D3BJ) = -2555.25268499
SCF(BS2) = -4338.47509891
SCF(BS2+D3BJ) = -
4338.81691529
Low Freq. = 16.0660cm-1,
19.5521cm-1

C -6.12460 0.03566 1.22484
C -5.26618 1.05494 0.70680
C -3.86834 0.75358 0.51280
C -3.37821 -0.55375 0.84363
C -4.25148 -1.52994 1.33845
C -5.62203 -1.22294 1.52718
C -2.98808 1.75854 -0.01967
C -3.49552 3.02370 -0.35019
C -4.86556 3.30701 -0.14914
C -5.73965 2.35634 0.36855
N -1.62944 1.45025 -0.20346
B -1.09136 0.17568 0.13322
N -2.00703 -0.79813 0.67244
Ni 0.78787 -0.24200 -0.02465
C 0.83676 -0.33626 -1.92389
N -0.06777 -0.70836 -2.90041
C 0.49111 -0.62665 -4.17652
C 1.77918 -0.20293 -4.02065
N 1.97646 -0.02948 -2.65094
C -1.40450 -1.22651 -2.69969
C -2.51161 -0.41845 -3.04729
C -3.79351 -0.98203 -2.90244
C -3.98958 -2.29814 -2.44733
C -2.85543 -3.07495 -2.14555
C -1.55084 -2.56486 -2.26594
C 3.27548 0.27650 -2.09027
C 3.72961 1.61693 -2.07615
C 5.02703 1.85254 -1.57979
C 5.86326 0.81430 -1.12961
C 5.38527 -0.50782 -1.20553
C 4.09974 -0.80500 -1.69441
C 2.88494 2.74844 -2.60299
C 7.24133 1.11106 -0.57806
C 3.64336 -2.24048 -1.84608
C -2.34770 0.98566 -3.58197
C -5.38474 -2.85060 -2.25564
C -0.35379 -3.43302 -1.94735
C 0.91421 -0.20260 1.87002
N 1.08309 -1.29364 2.71330
C 1.22129 -0.90091 4.04481
C 1.13053 0.46212 4.05983
N 0.94424 0.87115 2.74104
C 1.16703 -2.67711 2.30297
C 0.06844 -3.53466 2.53996
C 0.19171 -4.88146 2.14487
C 1.36789 -5.38507 1.56191
C 2.46032 -4.50936 1.40396
C 2.39168 -3.15585 1.77767
C 0.82515 2.27157 2.38797
C -0.40620 2.92577 2.61381
C -0.48068 4.29357 2.29834
C 0.62229 5.00523 1.79305
C 1.84024 4.32056 1.62965
C 1.97044 2.95189 1.91937
C -1.60006 2.20728 3.20220
C 0.49016 6.45609 1.39249
C 3.29699 2.24758 1.74453
C -1.17656 -3.06484 3.26199
C 1.46339 -6.82982 1.12097
C 3.61160 -2.26609 1.69057
Cl -0.41007 3.94847 -1.91598
H -1.07499 2.21061 -0.65151
H -1.70640 -1.75346 0.85144
H 1.37814 -1.62086 4.84341
H 1.18799 1.17703 4.87599
H -1.43527 4.81292 2.44099
H 2.71572 4.86365 1.25505
H 3.55763 1.63620 2.62619
H 4.10360 2.97967 1.58377
H 3.28543 1.57367 0.86964
H 0.17342 6.51863 0.33571
H 1.44817 6.99405 1.48637
H -0.26645 6.98009 1.99973
H -1.70817 1.18800 2.79889
H -2.52699 2.75721 2.98041
H -1.51702 2.11965 4.30172
H -0.65564 -5.55656 2.31416
H 3.40310 -4.89515 0.99824
H 3.47555 -1.42249 0.99265
H 4.48670 -2.84166 1.35194
H 3.85264 -1.82689 2.67475
H 0.74696 -7.46686 1.66434
H 2.47645 -7.23434 1.28178
H 1.24134 -6.93070 0.04281
H -1.03791 -3.11949 4.35750
H -2.03763 -3.70621 3.01557
H -1.43577 -2.02101 3.02583
H -0.07888 -0.87950 -5.06599
H 2.56719 -0.01017 -4.74355
H 5.39547 2.88506 -1.56038
H 6.03703 -1.33517 -0.90023
H 2.76072 -2.46563 -1.22220
H 4.44847 -2.93566 -1.56157
H 3.35710 -2.45966 -2.88993
H 7.67923 2.00743 -1.04706
H 7.93157 0.26607 -0.73626
H 7.20054 1.30078 0.51038
H 2.63005 2.59694 -3.66677
H 3.42498 3.70453 -2.52106
H 1.91711 2.86083 -2.07682
H -4.66455 -0.36478 -3.15065

H -2.98689 -4.11210 -1.81322
H 0.38168 -3.43253 -2.77094
H -0.66628 -4.47378 -1.76747
H 0.17744 -3.07293 -1.04686
H -6.08088 -2.46998 -3.02148
H -5.78291 -2.54640 -1.27031
H -5.39477 -3.95252 -2.29508
H -1.61275 1.57918 -3.01158
H -3.30803 1.52218 -3.54624
H -2.01012 0.97821 -4.63494
H -2.81155 3.76469 -0.77823
H -5.24086 4.30238 -0.41393
H -6.79998 2.58921 0.51653
H -3.86925 -2.52803 1.57841
H -6.28922 -1.99699 1.92350
H -7.18500 0.26527 1.37621

3
SCF = -2554.93220797
H(0 K)= -2553.993012
H(298 K)= -2553.929480
G(298 K)= -2554.092317
SCF(D3BJ) = -2555.27648801
SCF(BS2) = -4338.50084996
SCF(BS2+D3BJ) = -
4338.84513007
Low Freq. = 7.0957cm-1,
17.4320cm-1

Ni -0.00032 -0.98039 0.00024
Cl -0.00080 -3.33973 0.00082
N 1.01416 -0.88402 -2.80045
N -1.13387 -1.19034 -2.75665
N -1.01502 -0.88178 2.80081
N 1.13288 -1.18914 2.75753
N -1.20070 1.75232 0.10863
H -2.10408 1.29532 0.23078
N 1.20245 1.75121 -0.10911
H 2.10540 1.29332 -0.23105
C -0.05428 -0.95065 -1.91373
C 0.61071 -1.10124 -4.12226
H 1.32206 -1.09868 -4.94356
C -0.73700 -1.29174 -4.09446
H -1.45335 -1.48644 -4.88802
C -2.54331 -1.24134 -2.41751
C -3.28117 -0.03249 -2.44587
C -4.66409 -0.09502 -2.19227
H -5.24324 0.83641 -2.21071
C -5.32416 -1.31547 -1.96010
C -4.56739 -2.49886 -2.01935
H -5.07157 -3.46502 -1.89556
C -3.18055 -2.49621 -2.26518
C -2.43468 -3.79820 -2.42787
H -1.99175 -3.88032 -3.43704
H -3.11560 -4.65272 -2.28633
H -1.60552 -3.87509 -1.70208
C -6.80981 -1.35533 -1.67296
H -7.00768 -1.24182 -0.59118
H -7.25735 -2.31261 -1.98758
H -7.34421 -0.53941 -2.18787
C -2.64076 1.27805 -2.84562
H -1.67734 1.43778 -2.33970
H -3.29746 2.12795 -2.60231
H -2.45172 1.30209 -3.93484
C 2.37947 -0.49142 -2.51645
C 2.75430 0.84499 -2.80405
C 4.09803 1.21260 -2.60059
H 4.39659 2.24582 -2.81501
C 5.06355 0.29028 -2.15666
C 4.65884 -1.03805 -1.93354
H 5.40280 -1.78238 -1.62597
C 3.32830 -1.46193 -2.11772
C 2.95706 -2.91488 -1.95479
H 2.15972 -3.05520 -1.20373
H 3.83594 -3.50766 -1.65575
H 2.56979 -3.33149 -2.90250
C 6.49765 0.71824 -1.92881
H 6.78177 1.55210 -2.59200
H 7.19990 -0.11394 -2.10338
H 6.65017 1.06225 -0.88926
C 1.77198 1.84916 -3.36628
H 1.60860 1.68493 -4.44711
H 2.14818 2.87528 -3.23438
H 0.79105 1.78046 -2.87183
C 0.05354 -0.94945 1.91429
C -0.61187 -1.09843 4.12280
H -1.32336 -1.09505 4.94399
C 0.73575 -1.28955 4.09533
H 1.45189 -1.48403 4.88914
C 2.54232 -1.24087 2.41855
C 3.17905 -2.49607 2.26676
C 4.56587 -2.49938 2.02085
H 5.06965 -3.46580 1.89745
C 5.32310 -1.31631 1.96101
C 4.66356 -0.09550 2.19275
H 5.24310 0.83570 2.21076
C 3.28068 -0.03231 2.44642
C 2.64083 1.27863 2.84576
H 1.67741 1.43851 2.33991
H 3.29782 2.12819 2.60202
H 2.45195 1.30316 3.93500
C 6.80870 -1.35693 1.67369
H 7.25618 -2.31363 1.99015
H 7.34329 -0.54003 2.18684
H 7.00638 -1.24567 0.59164
C 2.43264 -3.79766 2.43010
H 1.98939 -3.87893 3.43919
H 3.11329 -4.65254 2.28934
H 1.60367 -3.87472 1.70412
C -2.38014 -0.48885 2.51636
C -3.32927 -1.45924 2.11803
C -4.65960 -1.03497 1.93337
H -5.40379 -1.77919 1.62610
C -5.06386 0.29365 2.15564
C -4.09809 1.21586 2.59927
H -4.39632 2.24930 2.81308
C -2.75454 0.84785 2.80320
C -1.77203 1.85194 3.36526
H -1.61009 1.68894 4.44649
H -2.14726 2.87820 3.23166
H -0.79060 1.78185 2.87204
C -6.49775 0.72200 1.92717

H	-7.20035	-0.10980	2.10214
H	-6.64985	1.06532	0.88733
H	-6.78172	1.55644	2.58968
C	-2.95856	-2.91244	1.95612
H	-2.16104	-3.05357	1.20541
H	-3.83759	-3.50504	1.65714
H	-2.57181	-3.32862	2.90422
C	-1.23960	3.14906	0.10598
C	-2.44411	3.86117	0.20561
H	-3.38728	3.31061	0.29032
C	-2.43346	5.27615	0.20378
H	-3.38574	5.81294	0.28325
C	-1.24564	5.99086	0.10350
H	-1.24996	7.08614	0.10330
C	0.00243	5.30511	-0.00131
C	0.00180	3.86329	-0.00086
C	1.24258	3.14792	-0.10727
C	2.44771	3.85891	-0.20730
H	3.39040	3.30748	-0.29163
C	2.43829	5.27389	-0.20636
H	3.39103	5.80981	-0.28614
C	1.25109	5.98971	-0.10655
H	1.25636	7.08498	-0.10704
B	0.00053	0.94914	-0.00007

Int(1-4)1

SCF = -2540.42698316
H(0 K)= -2539.483086
H(298 K)= -2539.420035
G(298 K)= -2539.583721
SCF(D3BJ) = -2540.75269247
SCF(BS2) = -3878.77146572
SCF(BS2+D3BJ) = -3879.09717498
Low Freq. = 14.6883cm-1, 17.6519cm-1

Ni	0.50877	-0.06374	-0.00722
N	1.42789	-0.17657	-2.79585
N	-0.68275	-0.68320	-2.68793
N	1.87056	0.02431	2.63777
N	1.01583	-1.94585	2.37520
C	0.39500	-0.33491	-1.85395
C	1.00303	-0.42795	-4.10871
H	1.67913	-0.34885	-4.95612
C	-0.31826	-0.74506	-4.03924
H	-1.03190	-1.01225	-4.81422
C	2.80538	0.13490	-2.52089
C	3.76154	-0.90738	-2.59549
C	5.12185	-0.57526	-2.45610
H	5.86858	-1.37693	-2.51531
C	5.54738	0.75117	-2.25653
C	4.56809	1.75950	-2.18574
H	4.87881	2.80084	-2.03672
C	3.19514	1.47872	-2.31375
C	3.33638	-2.33779	-2.84438
H	3.06636	-2.50491	-3.90315
H	2.44871	-2.59759	-2.24478
H	4.15093	-3.03627	-2.59439
C	7.01733	1.08038	-2.09829
H	7.64854	0.42510	-2.72171
H	7.34836	0.94614	-1.05147
H	7.22897	2.12611	-2.37596
C	2.16950	2.58528	-2.23926
H	1.47031	2.54567	-3.09239
H	2.65524	3.57380	-2.22711
H	1.56588	2.47649	-1.31928
C	-2.03842	-0.92195	-2.26713
C	-2.35465	-2.13950	-1.62367
C	-3.69043	-2.35787	-1.23855
H	-3.94410	-3.29733	-0.73171
C	-4.70460	-1.41730	-1.49743
C	-4.35910	-0.24117	-2.18834
H	-5.13611	0.49940	-2.41227
C	-3.03743	0.02862	-2.58735
C	-1.29152	-3.18450	-1.39542
H	-0.49899	-2.79855	-0.72918
H	-0.80034	-3.46381	-2.34508
H	-1.71854	-4.09191	-0.94293
C	-6.12604	-1.64828	-1.03044
H	-6.29748	-2.70299	-0.75870
H	-6.85946	-1.37020	-1.80683
H	-6.34767	-1.03099	-0.14075
C	-2.71455	1.28589	-3.36397
H	-2.64290	1.08439	-4.44893
H	-1.74955	1.71104	-3.04698
H	-3.49421	2.04813	-3.21291
C	1.17837	-0.73929	1.68579
C	1.57335	-1.91520	3.66091
H	1.53748	-2.77573	4.32404
C	2.11300	-0.67398	3.82299
H	2.65052	-0.22889	4.65662
C	2.34789	1.37311	2.45214
C	1.63870	2.44562	3.04436
C	2.16286	3.74275	2.89554
H	1.62132	4.58209	3.34894
C	3.35751	3.99046	2.19282
C	4.04698	2.89251	1.64663
H	4.99399	3.05895	1.11918
C	3.56828	1.57456	1.76898
C	0.35815	2.21784	3.81596
H	-0.43523	1.82188	3.15756
H	-0.00388	3.16106	4.25455
H	0.49379	1.48969	4.63470
C	3.88112	5.40189	2.02761
H	4.95988	5.40873	1.80066
H	3.71759	6.00340	2.93773
H	3.36717	5.92427	1.19968
C	4.35067	0.41100	1.20745
H	4.47275	-0.39083	1.95642
H	5.35027	0.73590	0.88017
H	3.83248	-0.03210	0.33952
C	0.48289	-3.18677	1.86420
C	-0.82102	-3.59240	2.22446
C	-1.24019	-4.88440	1.84766
H	-2.24704	-5.21382	2.13237
C	-0.40980	-5.75913	1.12688
C	0.88319	-5.31609	0.78270
H	1.55359	-5.98757	0.23233
C	1.35619	-4.04596	1.15125
C	-1.77078	-2.68088	2.97011
H	-1.24327	-1.97573	3.63131

H	-2.47963	-3.26438	3.57998
H	-2.37020	-2.08910	2.25379
C	-0.88971	-7.13614	0.71861
H	-1.78859	-7.43445	1.28221
H	-0.11149	-7.90074	0.88414
H	-1.14715	-7.16668	-0.35599
C	2.76687	-3.61468	0.82466
H	2.76605	-2.66231	0.26624
H	3.28295	-4.38076	0.22469
H	3.35687	-3.44512	1.74368
H	0.26515	1.42759	0.69593
C	-4.37217	4.74404	-1.10644
H	-4.63378	5.62272	-1.70705
C	-5.33798	4.13789	-0.31188
H	-6.36140	4.52695	-0.27988
C	-5.00803	2.99605	0.48012
C	-5.59263	1.24157	2.07955
H	-6.33147	0.75228	2.72469
C	-5.96367	2.34366	1.31714
H	-6.98821	2.72943	1.35202
H	-3.99416	-0.12445	2.66569
C	-4.27142	0.73852	2.05028
C	-3.30169	1.34774	1.23987
C	-3.66065	2.48602	0.43576
C	-2.68248	3.12646	-0.40239
C	-3.04818	4.24938	-1.16001
H	-2.29953	4.73970	-1.79284
N	-1.98131	0.90781	1.20387
H	-1.76205	0.09202	1.77518
B	-0.94607	1.45519	0.34212
N	-1.39100	2.60303	-0.42897
H	-0.73047	3.10324	-1.02093

^{3}Int(1-4)1

SCF = -2540.38213755
H(0 K)= -2539.439543
H(298 K)= -2539.376496
G(298 K)= -2539.541504
SCF(D3BJ) = -2540.70564171
SCF(BS2) = -3878.72320068
SCF(BS2+D3BJ) = -3879.04656301
Low Freq. = 12.9280cm-1, 17.1162cm-1

Ni	-0.18932	-0.53908	0.03570
N	0.38713	-1.08859	-2.82136
N	-1.41002	0.14128	-2.65547
N	0.90973	-1.20236	2.77001
N	-1.26164	-1.41787	2.69934
C	-0.47201	-0.53457	-1.86461
C	-0.00102	-0.74798	-4.12692
H	0.53899	-1.10962	-4.99817
C	-1.12351	0.01749	-4.01924
H	-1.75588	0.46817	-4.77968
C	1.33637	-2.15976	-2.59901
C	0.83560	-3.48299	-2.46580
C	1.75568	-4.54056	-2.39105
H	1.37077	-5.56261	-2.28617
C	3.14742	-4.33048	-2.47250
C	3.60552	-3.00964	-2.62286
H	4.68378	-2.82080	-2.69348
C	2.72692	-1.91109	-2.69357
C	-0.64846	-3.75571	-2.41376
H	-1.16745	-3.34097	-3.29638
H	-1.10257	-3.27809	-1.52596
H	-0.84730	-4.83843	-2.37491
C	4.11136	-5.49785	-2.44160
H	4.11968	-6.03730	-3.40713
H	3.83347	-6.23305	-1.66698
H	5.14311	-5.16529	-2.24243
C	3.28338	-0.51322	-2.83484
H	2.74799	0.07412	-3.60086
H	4.34768	-0.54265	-3.11704
H	3.20646	0.03412	-1.87772
C	-2.56915	0.86411	-2.19343
C	-3.68093	0.14175	-1.69949
C	-4.82810	0.86640	-1.32571
H	-5.69653	0.31153	-0.95166
C	-4.89715	2.26684	-1.43107
C	-3.77572	2.94756	-1.93891
H	-3.80823	4.03939	-2.03796
C	-2.60476	2.27427	-2.33120
C	-3.66727	-1.36586	-1.60346
H	-3.02768	-1.70999	-0.77107
H	-3.27270	-1.82613	-2.52522
H	-4.68301	-1.75284	-1.42753
C	-6.13442	3.02418	-0.99699
H	-7.03619	2.39201	-1.05169
H	-6.30204	3.91704	-1.62223
H	-6.04183	3.37469	0.04770
C	-1.43662	3.05076	-2.89369
H	-1.30989	2.87881	-3.97825
H	-0.49486	2.75799	-2.40391
H	-1.58154	4.13171	-2.74337
C	-0.17875	-1.04171	1.89102
C	-0.85700	-1.79600	3.98366
H	-1.57085	-2.11043	4.74063
C	0.49787	-1.66069	4.02782
H	1.21015	-1.85100	4.82621
C	2.31046	-1.04820	2.45985
C	3.05862	-0.01657	3.07648
C	4.43650	0.06333	2.78930
H	5.02094	0.86773	3.25306
C	5.07745	-0.84285	1.92972
C	4.30750	-1.88506	1.37207
H	4.79230	-2.62700	0.72613
C	2.93569	-2.01883	1.63201
C	2.45358	0.99397	4.03000
H	2.59971	2.02240	3.65659
H	2.93971	0.93740	5.02065
H	1.37581	0.83523	4.18548
C	6.55048	-0.70900	1.60645
H	7.04506	-1.69435	1.55611
H	7.07658	-0.09915	2.35906
H	6.70124	-0.22127	0.62567
C	2.15298	-3.17542	1.06391
H	1.62646	-3.73337	1.85912
H	2.81352	-3.87041	0.52354
H	1.37702	-2.81397	0.36040
C	-2.64256	-1.49540	2.29971
C	-3.42214	-0.31616	2.23871

C	-4.79661	-0.45021	1.97106
H	-5.41317	0.45565	1.93617
C	-5.40218	-1.70492	1.76747
C	-4.59069	-2.85308	1.82502
H	-5.04180	-3.84023	1.66509
C	-3.21033	-2.77576	2.08589
C	-2.80521	1.04144	2.47799
H	-2.27677	1.07651	3.44734
H	-3.57401	1.82961	2.47426
H	-2.05965	1.27473	1.69551
C	-6.88279	-1.81408	1.46881
H	-7.44978	-0.98764	1.92855
H	-7.30139	-2.76526	1.83750
H	-7.07692	-1.77596	0.38025
C	-2.36644	-4.03079	2.15185
H	-1.42327	-3.90770	1.59368
H	-2.91365	-4.88906	1.73057
H	-2.09026	-4.28783	3.19079
H	1.40180	0.01580	0.09514
C	2.65946	5.33230	-2.22688
H	3.04506	5.81377	-3.13306
C	2.51548	6.07325	-1.05927
H	2.78193	7.13538	-1.03313
C	2.01733	5.45550	0.12859
C	1.35357	5.53234	2.47962
H	1.22046	6.09392	3.41161
C	1.84783	6.17588	1.35066
H	2.10909	7.23916	1.38016
H	0.62197	3.67235	3.35619
C	1.01669	4.15927	2.45735
C	1.17939	3.40773	1.28045
C	1.67335	4.05769	0.09234
C	1.82119	3.31461	-1.13198
C	2.31447	3.96216	-2.27674
H	2.43043	3.39558	-3.20801
N	0.87947	2.05483	1.21887
H	0.51650	1.64309	2.07616
B	0.94422	1.22754	0.01384
N	1.45086	1.97486	-1.14308
H	1.58282	1.49562	-2.03179

^{3}TS(1-4)

SCF = -2540.37016023
H(0 K)= -2539.429838
H(298 K)= -2539.366973
G(298 K)= -2539.532146
SCF(D3BJ) = -2540.69168628
SCF(BS2) = -3878.71254052
SCF(BS2+D3BJ) = -3879.03406657
Low Freq. = -212.1922cm-1, 7.3707cm-1

Ni	-0.25682	-0.44745	0.00177
N	-0.37707	-1.47396	-2.78589
N	-1.55754	0.34133	-2.63497
N	0.79932	-1.20190	2.72530
N	-1.36241	-0.96780	2.75252
C	-0.80428	-0.53393	-1.84948
C	-0.85107	-1.19373	-4.07272
H	-0.62131	-1.83171	-4.92225
C	-1.59329	-0.05340	-3.97635
H	-2.15026	0.50382	-4.72520
C	0.30796	-2.71840	-2.50887
C	-0.46783	-3.84271	-2.13562
C	0.18475	-5.07947	-1.99061
H	-0.40772	-5.95484	-1.69703
C	1.56582	-5.22592	-2.22418
C	2.29935	-4.08589	-2.59888
H	3.37733	-4.17601	-2.78001
C	1.69561	-2.82365	-2.75178
C	-1.95546	-3.71952	-1.90003
H	-2.47948	-3.35127	-2.80022
H	-2.16500	-2.99698	-1.09116
H	-2.39099	-4.69306	-1.62496
C	2.23288	-6.58086	-2.11054
H	2.12837	-7.15771	-3.04835
H	1.78280	-7.18723	-1.30678
H	3.31169	-6.48477	-1.90545
C	2.52684	-1.61705	-3.11667
H	2.05644	-1.01117	-3.90988
H	3.53021	-1.91569	-3.45906
H	2.64711	-0.97241	-2.22614
C	-2.33634	1.46587	-2.16785
C	-3.56051	1.20989	-1.50894
C	-4.34632	2.31155	-1.12119
H	-5.29868	2.12245	-0.61164
C	-3.95800	3.63599	-1.38874
C	-2.75442	3.84563	-2.08706
H	-2.44463	4.86934	-2.32961
C	-1.92953	2.78197	-2.49588
C	-4.03649	-0.20075	-1.25512
H	-3.46325	-0.67477	-0.43928
H	-3.91156	-0.83432	-2.14993
H	-5.09918	-0.20625	-0.96849
C	-4.80763	4.80678	-0.94140
H	-5.85015	4.50184	-0.75290
H	-4.81617	5.61182	-1.69555
H	-4.41796	5.24727	-0.00524
C	-0.66019	3.06030	-3.26830
H	-0.65303	2.55428	-4.24966
H	0.22189	2.70457	-2.71101
H	-0.54344	4.14102	-3.44375
C	-0.26976	-0.87016	1.88131
C	-0.98279	-1.35120	4.04373
H	-1.70708	-1.47138	4.84532
C	0.37223	-1.49493	4.02447
H	1.07373	-1.77353	4.80632
C	2.19594	-1.32464	2.37231
C	3.11732	-0.35944	2.83454
C	4.48172	-0.54930	2.52873
H	5.20401	0.20188	2.87134
C	4.93861	-1.66448	1.81087
C	3.99221	-2.63141	1.41240
H	4.33092	-3.52855	0.87981
C	2.62359	-2.49033	1.68603
C	2.71385	0.83920	3.66644
H	3.04313	1.77946	3.19274
H	3.18563	0.79480	4.66498
H	1.62600	0.89687	3.81531
C	6.40466	-1.83122	1.47041
H	6.74027	-2.87142	1.62462

H	7.04003	-1.17124	2.08319
H	6.59768	-1.58347	0.41057
C	1.63847	-3.55657	1.27696
H	1.03529	-3.90095	2.13628
H	2.15647	-4.42586	0.84324
H	0.93740	-3.15242	0.52370
C	-2.75392	-0.79760	2.41621
C	-3.32146	0.49821	2.41324
C	-4.71199	0.60782	2.22893
H	-5.16361	1.60699	2.23987
C	-5.53503	-0.52018	2.04888
C	-4.93101	-1.79104	2.04655
H	-5.55404	-2.68296	1.90670
C	-3.54581	-1.95663	2.23070
C	-2.46859	1.72978	2.60696
H	-1.79645	1.62342	3.47613
H	-3.09485	2.62254	2.76021
H	-1.83375	1.90149	1.71823
C	-7.02650	-0.36677	1.83669
H	-7.42826	0.49363	2.39747
H	-7.57512	-1.26955	2.15166
H	-7.26342	-0.19725	0.76969
C	-2.92776	-3.33772	2.25274
H	-2.02248	-3.37972	1.62407
H	-3.64393	-4.09130	1.88872
H	-2.62035	-3.63111	3.27298
H	1.21837	-0.81658	-0.19961
C	4.23264	4.03582	-2.42592
H	4.83762	4.22644	-3.32006
C	4.32214	4.89592	-1.33678
H	4.99001	5.76379	-1.36175
C	3.54204	4.65689	-0.16495
C	2.81207	5.23359	2.09551
H	2.85511	5.89627	2.96772
C	3.59334	5.50985	0.97971
H	4.25518	6.38254	0.96111
H	1.34113	3.91065	3.02010
C	1.95569	4.10807	2.13443
C	1.87701	3.24038	1.03247
C	2.66788	3.51139	-0.13657
C	2.58647	2.64211	-1.27849
C	3.37186	2.91477	-2.41084
H	3.31252	2.24983	-3.28019
N	1.05002	2.11767	1.02665
H	0.51019	1.97447	1.87727
B	0.87785	1.18437	-0.08084
N	1.71156	1.56086	-1.22169
H	1.72249	0.95002	-2.03735

^{3}Int(1-4)2

SCF = -2540.37725538
H(0 K)= -2539.436162
H(298 K)= -2539.372872
G(298 K)= -2539.540741
SCF(D3BJ) = -2540.70415039
SCF(BS2) = -3878.71922221
SCF(BS2+D3BJ) = -3879.04582225
Low Freq. = 2.7696cm-1, 9.4716cm-1

Ni	-0.62415	0.15469	-0.05377
N	-1.98174	0.84979	-2.61390
N	0.01421	1.69306	-2.60141
N	-1.03544	-1.32195	2.53932
N	-0.83691	0.81400	2.86225
C	-0.86709	0.98519	-1.78553
C	-1.79029	1.44474	-3.86428
H	-2.56235	1.43681	-4.62942
C	-0.53331	1.97440	-3.85754
H	0.01907	2.52453	-4.61491
C	-3.25182	0.26704	-2.25039
C	-4.22686	1.09553	-1.64820
C	-5.48739	0.53725	-1.36859
H	-6.24979	1.16787	-0.89466
C	-5.79865	-0.79670	-1.69423
C	-4.80574	-1.58078	-2.31049
H	-5.02948	-2.62199	-2.57302
C	-3.52613	-1.07321	-2.60290
C	-3.93227	2.54706	-1.34209
H	-3.77517	3.12801	-2.26919
H	-3.01274	2.65067	-0.74137
H	-4.76704	3.00881	-0.79162
C	-7.17846	-1.35983	-1.42356
H	-7.87308	-1.13214	-2.25352
H	-7.61796	-0.93162	-0.50721
H	-7.15283	-2.45627	-1.31197
C	-2.47061	-1.94066	-3.24471
H	-2.05919	-1.48208	-4.16064
H	-2.87745	-2.93047	-3.50550
H	-1.63028	-2.07311	-2.53780
C	1.33875	2.14163	-2.24805
C	1.48136	3.30685	-1.46426
C	2.78758	3.75888	-1.18880
H	2.91331	4.66227	-0.57933
C	3.92531	3.10354	-1.69357
C	3.73672	1.95450	-2.48626
H	4.61105	1.42223	-2.87830
C	2.45656	1.45142	-2.77450
C	0.27536	4.05866	-0.95071
H	-0.30261	3.44933	-0.23399
H	-0.41153	4.32418	-1.77384
H	0.58163	4.98616	-0.44281
C	5.31995	3.61826	-1.40608
H	5.30362	4.45202	-0.68553
H	5.81252	3.98011	-2.32667
H	5.95939	2.81861	-0.99322
C	2.28501	0.19102	-3.59157
H	1.69110	0.36549	-4.50574
H	1.75542	-0.57905	-3.00322
H	3.26354	-0.21610	-3.88945
C	-0.86762	-0.12993	1.83222
C	-0.97950	0.23010	4.12598
H	-0.98759	0.82182	5.03775
C	-1.10306	-1.11188	3.92006
H	-1.23976	-1.93446	4.61701
C	-1.13150	-2.65460	1.99160
C	-0.01218	-3.51104	2.09170
C	-0.14566	-4.82803	1.60872
H	0.72015	-5.49830	1.66815
C	-1.35058	-5.30138	1.05910
C	-2.45197	-4.42446	1.01281

H	-3.40777	-4.78182	0.60997
C	-2.37059	-3.09961	1.47527
C	1.28514	-3.05075	2.71901
H	2.10862	-3.72920	2.44825
H	1.21553	-3.02895	3.82239
H	1.55448	-2.03510	2.38825
C	-1.46239	-6.71357	0.52264
H	-2.44855	-7.15419	0.74758
H	-0.68720	-7.37099	0.94922
H	-1.34289	-6.73486	-0.57640
C	-3.56742	-2.18208	1.42046
H	-3.75687	-1.70224	2.39672
H	-4.47256	-2.73447	1.12301
H	-3.39081	-1.37528	0.68675
C	-0.74278	2.24319	2.69772
C	0.50482	2.87668	2.89294
C	0.54985	4.28236	2.81673
H	1.51174	4.78681	2.97003
C	-0.59922	5.05254	2.56286
C	-1.82685	4.38285	2.38990
H	-2.73789	4.96709	2.21103
C	-1.92688	2.98206	2.46168
C	1.74644	2.07502	3.21283
H	1.83222	1.18861	2.56265
H	1.72975	1.70444	4.25409
H	2.65177	2.69150	3.09506
C	-0.52134	6.56147	2.46238
H	0.38413	6.95353	2.95346
H	-1.39927	7.04313	2.92515
H	-0.49306	6.89002	1.40696
C	-3.26249	2.28515	2.33536
H	-3.24499	1.53216	1.52859
H	-4.06493	3.00947	2.12511
H	-3.52095	1.74850	3.26599
H	-1.23376	-1.19661	-0.51312
C	3.97602	-4.68703	-0.94510
H	4.01913	-5.74292	-1.23704
C	5.14625	-4.01970	-0.59969
H	6.11166	-4.53719	-0.61599
C	5.10548	-2.64482	-0.21633
C	6.18165	-0.57527	0.51533
H	7.08648	-0.02312	0.79537
C	6.27635	-1.91274	0.14756
H	7.24617	-2.42198	0.13238
H	4.87883	1.14725	0.83898
C	4.93646	0.09452	0.54110
C	3.75996	-0.58741	0.19135
C	3.83126	-1.96951	-0.19515
C	2.63642	-2.68087	-0.56212
C	2.72241	-4.03329	-0.93132
H	1.80983	-4.57374	-1.20522
N	2.50692	0.03077	0.21330
H	2.53277	1.03306	0.39744
B	1.24531	-0.60420	-0.13983
N	1.42751	-1.99019	-0.53222
H	0.58756	-2.53138	-0.74095

4

SCF = -2540.42859288
H(0 K)= -2539.485198
H(298 K)= -2539.422778
G(298 K)= -2539.583886
SCF(D3BJ) = -2540.76229560
SCF(BS2) = -3878.77117735
SCF(BS2+D3BJ) = -3879.10488013
Low Freq. = 12.9086cm-1, 17.1170cm-1

Ni	-0.02391	-0.90273	0.00953
H	-0.05384	-2.45955	0.02407
N	-1.06437	-0.77289	2.77345
N	1.05120	-1.24864	2.73339
N	1.01190	-0.85537	-2.76105
N	-1.11589	-1.27042	-2.70223
N	1.24645	1.86816	-0.10151
H	2.13554	1.38688	-0.23217
N	-1.15355	1.93540	0.07895
H	-2.06850	1.50818	0.22124
C	-0.00568	-0.93941	1.88237
C	-0.67334	-0.98340	4.10270
H	-1.38033	-0.91185	4.92468
C	0.65467	-1.27862	4.07812
H	1.35543	-1.51629	4.87394
C	2.41952	-1.53049	2.36760
C	3.37824	-0.49403	2.47565
C	4.72590	-0.81549	2.23609
H	5.47778	-0.02109	2.32036
C	5.13471	-2.12450	1.91406
C	4.15297	-3.12835	1.83780
H	4.45388	-4.15837	1.61000
C	2.78976	-2.86147	2.07211
C	1.76127	-3.96721	2.04203
H	1.27482	-4.08831	3.02681
H	2.22533	-4.92848	1.76931
H	0.96346	-3.72883	1.31331
C	6.59625	-2.43857	1.67042
H	6.96194	-1.95833	0.74461
H	6.76592	-3.52306	1.57327
H	7.23095	-2.06720	2.49400
C	2.97381	0.90682	2.87697
H	2.19809	1.30983	2.20388
H	3.84069	1.58585	2.85552
H	2.55259	0.92767	3.89814
C	-2.41522	-0.38972	2.44496
C	-2.83842	0.92638	2.74721
C	-4.17841	1.26593	2.47242
H	-4.51734	2.28506	2.69476
C	-5.08753	0.33755	1.93418
C	-4.63325	-0.97096	1.68116
H	-5.33030	-1.71551	1.27974
C	-3.30661	-1.36283	1.93431
C	-2.85577	-2.78682	1.71235
H	-1.98998	-2.82180	1.02544
H	-3.67179	-3.39197	1.28812
H	-2.53487	-3.25235	2.66230
C	-6.51532	0.73451	1.62342
H	-6.80411	1.65764	2.15191
H	-7.22641	-0.05994	1.90736
H	-6.65021	0.91722	0.54138
C	-1.90435	1.94190	3.36871
H	-1.77474	1.76196	4.45157

H	-2.30076	2.96152	3.24332
H	-0.90500	1.90434	2.90772
C	-0.04640	-0.97525	-1.86198
C	0.60797	-1.07902	-4.08441
H	1.31235	-1.04239	-4.91091
C	-0.72762	-1.33599	-4.04806
H	-1.43906	-1.56829	-4.83595
C	-2.48684	-1.52155	-2.32465
C	-2.88032	-2.84429	-2.01774
C	-4.24563	-3.08424	-1.77216
H	-4.56351	-4.10623	-1.53121
C	-5.20922	-2.06184	-1.84851
C	-4.77743	-0.76214	-2.17432
H	-5.51395	0.04739	-2.24866
C	-3.42531	-0.46775	-2.42818
C	-2.99863	0.92402	-2.83808
H	-2.19127	1.30709	-2.19137
H	-3.84749	1.62401	-2.78784
H	-2.61154	0.93691	-3.87296
C	-6.67898	-2.36009	-1.63473
H	-7.19497	-2.53137	-2.59770
H	-7.19521	-1.52187	-1.13747
H	-6.82416	-3.26525	-1.02231
C	-1.87104	-3.96725	-1.97942
H	-1.38842	-4.10602	-2.96372
H	-2.35120	-4.91762	-1.69659
H	-1.06841	-3.73532	-1.25388
C	2.37656	-0.51000	-2.44842
C	3.23969	-1.50141	-1.92457
C	4.58056	-1.14770	-1.69001
H	5.25675	-1.90737	-1.28091
C	5.07590	0.13907	-1.97490
C	4.19300	1.08564	-2.52541
H	4.56288	2.08827	-2.77171
C	2.84018	0.78494	-2.78096
C	1.93299	1.81814	-3.41265
H	1.79047	1.62539	-4.49171
H	2.36045	2.82717	-3.30565
H	0.93622	1.81677	-2.94465
C	6.51871	0.49564	-1.68517
H	7.19809	-0.33826	-1.93127
H	6.66426	0.72627	-0.61375
H	6.84076	1.38031	-2.25844
C	2.74655	-2.90593	-1.67100
H	1.89501	-2.90256	-0.96611
H	3.55107	-3.53209	-1.25525
H	2.38996	-3.37439	-2.60654
C	1.32548	3.26228	-0.12501
C	2.54945	3.94079	-0.23312
H	3.47825	3.36387	-0.30241
C	2.57781	5.35486	-0.25216
H	3.54480	5.86414	-0.33780
C	1.41016	6.10421	-0.16283
H	1.44513	7.19898	-0.17691
C	0.14344	5.45460	-0.05053
C	0.10434	4.01328	-0.03401
C	-1.15582	3.33213	0.07361
C	-2.34072	4.07868	0.16882
H	-3.29932	3.55474	0.25361
C	-2.29237	5.49223	0.15472
H	-3.23009	6.05515	0.22925
C	-1.08587	6.17457	0.04652
H	-1.06115	7.26964	0.03479
B	0.02435	1.08225	-0.00478

^{3}Int(1-3)1

SCF = -2554.84525780
H(0 K)= -2553.909834
H(298 K)= -2553.844827
G(298 K)= -2554.014006
SCF(D3BJ) = -2555.18115483
SCF(BS2) = -4338.40838552
SCF(BS2+D3BJ) = -4338.74459176
Low Freq. = 14.4267cm-1, 16.3107cm-1

C	-4.71265	4.26585	-0.49839
C	-3.32518	4.59158	-0.41452
C	-2.35542	3.53642	-0.55363
C	-2.79094	2.19080	-0.81092
C	-4.17241	1.91241	-0.87321
C	-5.11449	2.95067	-0.71975
C	-0.95041	3.82815	-0.45191
C	-0.54603	5.17021	-0.28324
C	-1.50378	6.19867	-0.16288
C	-2.86927	5.92839	-0.21032
N	-0.04906	2.78465	-0.50559
B	-0.36614	1.41228	-0.97587
N	-1.83742	1.20314	-1.00235
Ni	0.40688	-0.36501	-0.01185
C	0.36260	-1.68586	-1.45852
N	-0.68632	-2.17573	-2.24248
C	-0.22581	-2.96271	-3.30420
C	1.13090	-2.99353	-3.21398
N	1.47915	-2.22946	-2.09473
C	-2.10411	-2.05288	-2.00239
C	-2.91499	-1.37683	-2.95108
C	-4.30730	-1.36032	-2.72928
C	-4.90215	-1.99446	-1.62333
C	-4.06485	-2.68650	-0.72819
C	-2.67119	-2.74779	-0.90423
C	2.84679	-2.24747	-1.62438
C	3.82460	-1.48421	-2.30487
C	5.16978	-1.64467	-1.91561
C	5.55722	-2.53705	-0.90074
C	4.55483	-3.29376	-0.26266
C	3.19860	-3.17777	-0.61359
C	3.45980	-0.56457	-3.44604
C	7.00903	-2.67445	-0.49299
C	2.15739	-4.05954	0.03622
C	-2.33634	-0.70142	-4.17451
C	-6.39805	-1.93194	-1.39858
C	-1.81978	-3.58520	0.01856
C	0.72841	0.17367	1.84764
N	0.07247	-0.31171	2.97855
C	0.54267	0.27087	4.15952
C	1.51726	1.15015	3.79916
N	1.61630	1.09726	2.40554
C	-0.93191	-1.34757	3.04145
C	-2.29141	-1.00254	2.86320
C	-3.25448	-2.00618	3.08103

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C  -2.90156 -3.30952  3.47833
C  -1.53681 -3.60857  3.65029
C  -0.53294 -2.64525  3.44162
C   2.51521  1.97826  1.70082
C   2.27439  3.37365  1.74856
C   3.17895  4.21822  1.07606
C   4.29910  3.71842  0.38471
C   4.52838  2.33081  0.41028
C   3.66112  1.44212  1.07260
C   1.10491  3.96064  2.50902
C   5.22460  4.64724 -0.37111
C   3.98242 -0.02930  1.16170
C  -2.70090  0.40313  2.49139
C  -3.96127 -4.36906  3.69636
C   0.92353 -2.98131  3.67625
Cl  0.42304  1.36929 -2.95839
H   0.93049  3.06439 -0.46253
H  -2.21126  0.30552 -1.31410
H   0.13789  0.00341  5.13188
H   2.15059  1.80152  4.39467
H   3.00053  5.30015  1.09893
H   5.41656  1.92277 -0.08658
H   3.95140 -0.37876  2.20886
H   4.98271 -0.23502  0.75377
H   3.26102 -0.64581  0.59901
H   4.88364  4.77906 -1.41440
H   6.25203  4.24929 -0.41177
H   5.25944  5.64834  0.08956
H   0.18982  3.36571  2.36399
H   0.89692  4.98647  2.17015
H   1.30639  4.00279  3.59464
H  -4.31348 -1.75041  2.95661
H  -1.24172 -4.61673  3.96583
H   1.55935 -2.60583  2.85730
H   1.06407 -4.07053  3.75875
H   1.30026 -2.52302  4.60868
H  -4.92125 -3.92284  4.00389
H  -3.65513 -5.09448  4.46815
H  -4.15031 -4.94273  2.76970
H  -2.31850  1.13842  3.22123
H  -3.79708  0.49537  2.45465
H  -2.29835  0.69347  1.50568
H  -0.90856 -3.43796 -4.00270
H   1.88001 -3.49632 -3.81956
H   5.93660 -1.05921 -2.43744
H   4.83681 -4.01385  0.51531
H   1.36895 -3.45745  0.52012
H   2.61697 -4.71589  0.79183
H   1.65432 -4.69845 -0.71209
H   7.68772 -2.35363 -1.29999
H   7.25714 -3.71596 -0.22782
H   7.23594 -2.05328  0.39337
H   3.23532 -1.13916 -4.36415
H   4.29583  0.11432 -3.67862
H   2.56218  0.03724 -3.22101
H  -4.94191 -0.83404 -3.45207
H  -4.50781 -3.21983  0.12125
H  -1.15565 -4.25520 -0.55471
H  -2.45148 -4.19894  0.67785
H  -1.17067 -2.95976  0.65547
H  -6.94236 -1.76782 -2.34280
H  -6.66404 -1.10165 -0.71867
H  -6.77614 -2.86042 -0.93887
H  -1.42955 -0.12118 -3.93090
H  -3.07791 -0.01920 -4.61937
H  -2.05863 -1.43810 -4.95047
H   0.52402  5.40297 -0.25364
H  -1.15848  7.23072 -0.03052
H  -3.60551  6.73296 -0.10990
H  -4.49970  0.88502 -1.06463
H  -6.18259  2.71245 -0.78363
H  -5.45275  5.06633 -0.39110
```

^{3}TS(1-3)

SCF = -2554.84494432
H(0 K)= -2553.908785
H(298 K)= -2553.844852
G(298 K)= -2554.011962
SCF(D3BJ) = -2555.18027390
SCF(BS2) = -4338.40712151
SCF(BS2+D3BJ) = -4338.74245112
Low Freq. = -60.5806cm-1, 5.4390cm-1

```
C  -4.83136  4.31533 -0.54594
C  -3.44501  4.61644 -0.38909
C  -2.49029  3.54085 -0.45798
C  -2.93731  2.20073 -0.71635
C  -4.31754  1.94675 -0.85535
C  -5.24621  3.00443 -0.77065
C  -1.08919  3.80721 -0.28080
C  -0.66518  5.14272 -0.10900
C  -1.60649  6.19116 -0.05755
C  -2.97273  5.94639 -0.17875
N  -0.20870  2.74348 -0.26606
B  -0.53247  1.37913 -0.72343
N  -1.99166  1.19249 -0.82948
Ni  0.40733 -0.37641  0.00409
C   0.39210 -1.63160 -1.51717
N  -0.65743 -2.11432 -2.29720
C  -0.20011 -2.83545 -3.40475
C   1.15935 -2.82822 -3.34534
N   1.50866 -2.10745 -2.19880
C  -2.07252 -2.03625 -2.02019
C  -2.91655 -1.31895 -2.90726
C  -4.30335 -1.34642 -2.65405
C  -4.85992 -2.06046 -1.57652
C  -3.98963 -2.79068 -0.74645
C  -2.59910 -2.81208 -0.95798
C   2.88801 -2.09212 -1.76138
C   3.81793 -1.25676 -2.42449
C   5.17610 -1.37714 -2.06673
C   5.62175 -2.29770 -1.10190
C   4.66582 -3.12652 -0.48342
C   3.29890 -3.05283 -0.80382
C   3.39252 -0.30320 -3.51505
C   7.08610 -2.38918 -0.72723
C   2.31077 -4.01079 -0.17825
C  -2.37594 -0.55353 -4.09292
C  -6.35111 -2.04060 -1.31587
C  -1.71018 -3.68987 -0.11048
```

C	0.75117	0.10029	1.87377
N	0.12325	-0.45141	2.98889
C	0.56934	0.11596	4.18686
C	1.49862	1.05240	3.85189
N	1.59575	1.04824	2.45689
C	-0.82469	-1.54069	3.01692
C	-2.20517	-1.25912	2.89020
C	-3.10846	-2.32387	3.07019
C	-2.67797	-3.62732	3.38251
C	-1.29608	-3.86109	3.51014
C	-0.34931	-2.83467	3.33739
C	2.46562	1.97640	1.77623
C	2.20150	3.36472	1.88349
C	3.07813	4.25100	1.22704
C	4.19240	3.79969	0.49530
C	4.44743	2.41659	0.46332
C	3.61025	1.48709	1.10678
C	1.03790	3.90574	2.68726
C	5.08535	4.77259	-0.24360
C	3.96241	0.02044	1.13367
C	-2.69878	0.14197	2.61480
C	-3.67625	-4.75166	3.56243
C	1.12695	-3.10360	3.53207
Cl	0.33351	1.51500	-2.89893
H	0.77436	3.00374	-0.19059
H	-2.36144	0.29171	-1.13633
H	0.18327	-0.20261	5.15142
H	2.10326	1.71289	4.46668
H	2.88018	5.32766	1.29399
H	5.33210	2.04448	-0.06675
H	3.95410	-0.36971	2.16684
H	4.96037	-0.14852	0.70380
H	3.24445	-0.58856	0.55842
H	4.75260	4.89245	-1.29087
H	6.13004	4.42072	-0.27243
H	5.06941	5.77183	0.22171
H	0.13513	3.28834	2.56098
H	0.79248	4.93089	2.37135
H	1.27102	3.93936	3.76692
H	-4.18219	-2.11814	2.98507
H	-0.94133	-4.86738	3.76384
H	1.72549	-2.69126	2.70278
H	1.32058	-4.18556	3.59974
H	1.50361	-2.63575	4.45958
H	-4.62039	-4.38728	4.00016
H	-3.27774	-5.54583	4.21476
H	-3.92867	-5.22213	2.59375
H	-2.31194	0.85721	3.36177
H	-3.79864	0.18088	2.64164
H	-2.36513	0.50225	1.62595
H	-0.88445	-3.29479	-4.11236
H	1.90991	-3.27404	-3.99224
H	5.90640	-0.73593	-2.57527
H	4.99321	-3.86961	0.25407
H	1.49511	-3.47099	0.33262
H	2.81136	-4.66705	0.55085
H	1.83676	-4.65053	-0.94480
H	7.73605	-2.05399	-1.55198
H	7.37125	-3.42069	-0.46092
H	7.31520	-1.75396	0.14855
H	3.16982	-0.84596	-4.45280
H	4.19773	0.41605	-3.73488
H	2.47777	0.25596	-3.24728
H	-4.96440	-0.79098	-3.32991
H	-4.40252	-3.38558	0.07686
H	-1.03060	-4.29071	-0.73926
H	-2.31440	-4.37503	0.50276
H	-1.07725	-3.09644	0.57138
H	-6.92319	-1.91415	-2.24963
H	-6.62672	-1.20306	-0.64874
H	-6.68797	-2.96994	-0.82740
H	-1.50124	0.06324	-3.81569
H	-3.15392	0.10735	-4.50657
H	-2.05509	-1.23430	-4.90231
H	0.40630	5.35329	-0.02490
H	-1.24889	7.21829	0.07904
H	-3.69621	6.76725	-0.13154
H	-4.65252	0.92257	-1.04992
H	-6.31351	2.78563	-0.89070
H	-5.56072	5.13080	-0.49179

^{3}Int(1-3)3

SCF = -2554.88147390
H(0 K)= -2553.943817
H(298 K)= -2553.879693
G(298 K)= -2554.045187
SCF(D3BJ) = -2555.21928280
SCF(BS2) = -4338.44485072
SCF(BS2+D3BJ) = -4338.78265961
Low Freq. = 14.8518cm-1, 15.8540cm-1

C	-6.49896	1.32050	0.84574
C	-5.49034	2.09286	0.19060
C	-4.14997	1.56521	0.12048
C	-3.85397	0.28493	0.70152
C	-4.87589	-0.44363	1.33207
C	-6.18787	0.08341	1.39890
C	-3.11627	2.31769	-0.53670
C	-3.42473	3.56159	-1.11153
C	-4.74070	4.07041	-1.03581
C	-5.75742	3.36372	-0.40094
N	-1.83374	1.77851	-0.57435
B	-1.44491	0.49988	-0.02426
N	-2.54461	-0.19180	0.61857
Ni	0.55986	-0.03875	-0.14186
C	0.74360	-1.38867	-1.64927
N	-0.22786	-1.83695	-2.52511
C	0.31041	-2.57264	-3.58350
C	1.65938	-2.60932	-3.38681
N	1.90823	-1.89311	-2.21348
C	-1.66362	-1.68214	-2.41611
C	-2.29762	-0.65292	-3.14637
C	-3.70343	-0.60087	-3.10886
C	-4.46906	-1.54093	-2.39541
C	-3.79416	-2.56524	-1.70473
C	-2.39159	-2.65761	-1.69810
C	3.24219	-1.85608	-1.65226
C	4.18555	-0.92714	-2.14890
C	5.49294	-0.98720	-1.62694
C	5.87694	-1.94098	-0.66695

```
C   4.91929 -2.88214 -0.24332
C   3.60056 -2.86984 -0.73231
C   3.82843  0.06746 -3.22704
C   7.28239 -1.95793 -0.10424
C   2.61536 -3.94650 -0.33358
C  -1.49848  0.34695 -3.94879
C  -5.97688 -1.43312 -2.34192
C  -1.69203 -3.76675 -0.94336
C   1.05688  0.69105  1.65254
N   0.72755  0.08789  2.86724
C   1.07811  0.87460  3.96650
C   1.64032  2.00874  3.46313
N   1.62368  1.89027  2.06841
C   0.13302 -1.21527  3.02469
C  -1.21586 -1.31682  3.43934
C  -1.75773 -2.60933  3.59264
C  -0.99489 -3.77196  3.37629
C   0.36373 -3.62288  3.03423
C   0.95482 -2.35703  2.87020
C   2.22684  2.93812  1.27055
C   1.49947  4.12935  1.05520
C   2.14293  5.17328  0.36719
C   3.46614  5.05725 -0.09769
C   4.15988  3.86177  0.16172
C   3.56472  2.78822  0.84880
C   0.07231  4.28050  1.53189
C   4.11820  6.18455 -0.87013
C   4.33819  1.51799  1.11492
C  -2.04093 -0.09552  3.78208
C  -1.61284 -5.14676  3.51710
C   2.43886 -2.21266  2.62073
Cl  1.14980  1.74948 -1.60479
H  -1.11353  2.30714 -1.07800
H  -2.39877 -1.10790  1.04021
H   0.90019  0.54980  4.98808
H   2.05951  2.88312  3.95377
H   1.58909  6.10312  0.18801
H   5.19900  3.75873 -0.17451
H   4.23310  1.18598  2.16236
H   5.40976  1.66401  0.90481
H   3.97776  0.69374  0.47463
H   3.87993  6.11435 -1.94746
H   5.21652  6.15857 -0.77561
H   3.76588  7.17062 -0.52357
H  -0.58078  3.51617  1.07549
H  -0.32300  5.27349  1.26606
H  -0.01436  4.16309  2.62683
H  -2.80368 -2.70412  3.90902
H   0.98996 -4.51559  2.91782
H   2.65166 -1.72301  1.65579
H   2.93446 -3.19567  2.62748
H   2.90604 -1.58810  3.40285
H  -2.46662 -5.13721  4.21413
H  -0.87838 -5.88409  3.88145
H  -1.98813 -5.51562  2.54478
H  -1.89764  0.18495  4.84223
H  -3.11527 -0.28885  3.63465
H  -1.76525  0.77198  3.16548
H  -0.31644 -2.99582 -4.36386
H   2.45862 -3.07592 -3.95677
H   6.23538 -0.27028 -1.99755
H   5.20981 -3.66212  0.47090
H   1.70901 -3.52435  0.13247
H   3.07441 -4.65089  0.37774
H   2.28089 -4.52371 -1.21425
H   8.00704 -1.52456 -0.81291
H   7.60860 -2.98296  0.13879
H   7.34396 -1.36759  0.82854
H   3.51892 -0.44330 -4.15671
H   4.69266  0.70808 -3.46403
H   2.98577  0.70866 -2.91007
H  -4.21315  0.19940 -3.65802
H  -4.37531 -3.31472 -1.15363
H  -0.99476 -4.32793 -1.58999
H  -2.42513 -4.47986 -0.53401
H  -1.09499 -3.36944 -0.10244
H  -6.38061 -0.94808 -3.24601
H  -6.28831 -0.82582 -1.47231
H  -6.45093 -2.42381 -2.23898
H  -0.73583  0.84282 -3.32201
H  -2.15947  1.11709 -4.37672
H  -0.96170 -0.14108 -4.78288
H  -2.63501  4.13124 -1.61373
H  -4.95835  5.04471 -1.48878
H  -6.77337  3.77025 -0.34907
H  -4.65035 -1.42763  1.75896
H  -6.96952 -0.50139  1.89781
H  -7.51759  1.71927  0.90381
```

1_gas

```
SCF  =       -2019.48339730
H(0 K)=      -2018.710685
H(298 K)=    -2018.657419
G(298 K)=    -2018.806652
SCF(D3BJ) =        -
2019.71877710
SCF(BS2) =   -3357.64931823
SCF(BS2+D3BJ) =    -
3357.88469804
Low Freq. = 8.6538cm-1,
12.6501cm-1

Ni  0.00000  0.00000 -0.00003
N   0.00000  1.08489 -2.71832
N   0.00000 -1.08489 -2.71832
N  -1.08488 -0.00000  2.71825
N   1.08488  0.00000  2.71825
C   0.00000  0.00000 -1.84184
C   0.00000  0.68315 -4.05950
H   0.00000  1.39995 -4.87682
C   0.00000 -0.68315 -4.05950
H   0.00000 -1.39995 -4.87682
C   0.00000 -2.46433 -2.30066
C  -1.23545 -3.12809 -2.12449
C  -1.20824 -4.48828 -1.76753
H  -2.16034 -5.01389 -1.62277
C   0.00000 -5.18773 -1.58925
C   1.20824 -4.48828 -1.76753
H   2.16034 -5.01389 -1.62277
C   1.23545 -3.12809 -2.12449
```

```
C   2.54231 -2.38479 -2.27757
H   2.62897 -1.90653 -3.26889
H   3.39956 -3.06432 -2.14660
H   2.61392 -1.57756 -1.52589
C   0.00000 -6.66240 -1.24385
H  -0.89243 -6.94114 -0.65899
H   0.89243 -6.94114 -0.65899
H   0.00000 -7.28842 -2.15586
C  -2.54231 -2.38479 -2.27757
H  -2.61392 -1.57756 -1.52589
H  -3.39956 -3.06432 -2.14660
H  -2.62897 -1.90653 -3.26889
C  -0.00000  2.46433 -2.30066
C  -1.23545  3.12809 -2.12449
C  -1.20824  4.48828 -1.76753
H  -2.16034  5.01389 -1.62277
C  -0.00000  5.18773 -1.58925
C   1.20824  4.48828 -1.76753
H   2.16034  5.01389 -1.62277
C   1.23545  3.12809 -2.12449
C   2.54231  2.38479 -2.27757
H   2.61392  1.57756 -1.52589
H   3.39956  3.06432 -2.14660
H   2.62897  1.90653 -3.26889
C  -0.00000  6.66240 -1.24385
H  -0.00000  7.28842 -2.15586
H   0.89243  6.94114 -0.65899
H  -0.89243  6.94114 -0.65899
C  -2.54231  2.38479 -2.27757
H  -2.62897  1.90653 -3.26889
H  -3.39956  3.06432 -2.14660
H  -2.61392  1.57756 -1.52589
C   0.00000  0.00000  1.84178
C  -0.68315 -0.00000  4.05944
H  -1.39996 -0.00000  4.87675
C   0.68315  0.00000  4.05944
H   1.39996  0.00000  4.87675
C   2.46432  0.00000  2.30062
C   3.12809 -1.23545  2.12446
C   4.48829 -1.20824  1.76756
H   5.01391 -2.16034  1.62285
C   5.18776  0.00000  1.58931
C   4.48829  1.20824  1.76756
H   5.01391  2.16034  1.62285
C   3.12809  1.23545  2.12446
C   2.38481  2.54232  2.27756
H   1.57763  2.61398  1.52584
H   3.06435  3.39956  2.14667
H   1.90649  2.62894  3.26886
C   6.66246  0.00000  1.24401
H   7.28853  0.00000  2.15597
H   6.94114  0.89241  0.65909
H   6.94114 -0.89241  0.65909
C   2.38481 -2.54232  2.27756
H   1.90649 -2.62894  3.26886
H   3.06435 -3.39956  2.14667
H   1.57763 -2.61398  1.52584
C  -2.46432 -0.00000  2.30062
C  -3.12809 -1.23545  2.12446
C  -4.48829 -1.20824  1.76756
H  -5.01391 -2.16034  1.62285
C  -5.18776 -0.00000  1.58931
C  -4.48829  1.20824  1.76756
H  -5.01391  2.16034  1.62285
C  -3.12809  1.23545  2.12446
C  -2.38481  2.54232  2.27756
H  -1.90649  2.62894  3.26886
H  -3.06435  3.39956  2.14667
H  -1.57763  2.61398  1.52584
C  -6.66246 -0.00000  1.24401
H  -7.28853 -0.00000  2.15597
H  -6.94114 -0.89241  0.65909
H  -6.94114  0.89241  0.65909
C  -2.38481 -2.54232  2.27756
H  -1.57763 -2.61398  1.52584
H  -3.06435 -3.39956  2.14667
H  -1.90649 -2.62894  3.26886
```

ClBdan_gas

```
SCF  =       -535.419960114
H(0 K)=      -535.257591
H(298 K)=    -535.246126
G(298 K)=    -535.293796
SCF(D3BJ) =        -
535.468898509
SCF(BS2) =   -980.834274009
SCF(BS2+D3BJ) =    -
980.883212405
Low Freq. = 84.1862cm-1,
133.8023cm-1

C   2.14686  2.44420  0.00000
H   2.68396  3.39853 -0.00000
C   2.85497  1.25122  0.00001
H   3.94979  1.25204  0.00004
C   2.16821  0.00000  0.00000
C   2.14686 -2.44420  0.00001
H   2.68397 -3.39852  0.00002
C   2.85497 -1.25121  0.00001
H   3.94979 -1.25203 -0.00001
H   0.18545 -3.40575  0.00003
C   0.73098 -2.45554  0.00002
C   0.02405 -1.25197 -0.00001
C   0.72743  0.00000 -0.00001
C   0.02404  1.25197  0.00001
C   0.73098  2.45554 -0.00001
H   0.18544  3.40575 -0.00003
N  -1.38281 -1.21863 -0.00005
H  -1.85498 -2.12064 -0.00031
B  -2.11327 -0.00001 -0.00002
N  -1.38281  1.21863  0.00000
H  -1.85499  2.12063  0.00036
Cl -3.90935 -0.00000  0.00001
```

Int(1-4)1_gas

SCF = -2554.88174458
H(0 K)= -2553.945178
H(298 K)= -2553.880637
G(298 K)= -2554.047276
SCF(D3BJ) = -2555.22439745
SCF(BS2) = -4338.45204044
SCF(BS2+D3BJ) = -4338.79482785
Low Freq. = 13.7546cm-1, 16.5324cm-1

C	-5.65574	2.11625	0.60244
C	-4.53612	2.97317	0.38152
C	-3.32054	2.40433	-0.14388
C	-3.27335	1.00972	-0.48734
C	-4.39590	0.20135	-0.24914
C	-5.57242	0.76336	0.29681
C	-2.17242	3.24178	-0.35826
C	-2.27530	4.62284	-0.12451
C	-3.47648	5.17282	0.37827
C	-4.58159	4.37480	0.64700
N	-0.99888	2.65378	-0.81471
B	-0.87394	1.25657	-1.21795
N	-2.11502	0.50374	-1.07943
Ni	0.47045	-0.23384	-0.12623
C	0.65760	-1.72749	-1.36977
N	-0.23684	-2.55191	-2.06576
C	0.41433	-3.48162	-2.88479
C	1.74909	-3.27743	-2.72492
N	1.88597	-2.22583	-1.81421
C	-1.67394	-2.64683	-1.94423
C	-2.48385	-2.27727	-3.04997
C	-3.86535	-2.53234	-2.96489
C	-4.44688	-3.14957	-1.84212
C	-3.60560	-3.51698	-0.77527
C	-2.21729	-3.28950	-0.80502
C	3.20616	-1.89086	-1.33189
C	4.04724	-1.07415	-2.12009
C	5.36959	-0.87751	-1.67850
C	5.86383	-1.47335	-0.50418
C	5.00653	-2.32023	0.22445
C	3.68190	-2.56125	-0.18045
C	3.55257	-0.44589	-3.40245
C	7.27902	-1.21078	-0.03444
C	2.80825	-3.55542	0.54897
C	-1.89897	-1.64207	-4.29189
C	-5.94050	-3.38578	-1.77748
C	-1.33135	-3.75432	0.32450
C	0.86806	0.74718	1.43433
N	0.82550	0.16613	2.71174
C	1.42664	0.96469	3.68912
C	1.85938	2.08914	3.06111
N	1.50723	1.97051	1.71145
C	0.21732	-1.08727	3.08475
C	-1.19470	-1.17644	3.15593
C	-1.75395	-2.36780	3.65119
C	-0.96022	-3.44734	4.08389
C	0.43750	-3.30781	4.02507
C	1.05116	-2.13500	3.54476
C	1.72047	3.09874	0.83740
C	1.07641	4.32337	1.14947
C	1.34958	5.43935	0.33404
C	2.22244	5.36997	-0.76707
C	2.85198	4.14026	-1.03165
C	2.63284	2.99927	-0.23814
C	0.10425	4.45926	2.30293
C	2.46066	6.57403	-1.65339
C	3.36575	1.71628	-0.51481
C	-2.07046	-0.01722	2.75081
C	-1.59544	-4.72564	4.58955
C	2.55873	-1.99718	3.57131
Cl	0.13971	1.10822	-2.82276
H	-0.22999	3.29682	-0.99648
H	-2.16677	-0.47369	-1.36757
H	1.47329	0.66107	4.73112
H	2.38803	2.96004	3.43739
H	0.85412	6.38973	0.56776
H	3.55177	4.06320	-1.87263
H	3.95873	1.39192	0.35879
H	4.04538	1.82885	-1.37270
H	2.65100	0.89458	-0.72531
H	1.79994	6.55351	-2.53965
H	3.49897	6.60288	-2.02456
H	2.26149	7.51692	-1.11791
H	-0.54316	3.57267	2.39082
H	-0.54633	5.33409	2.15424
H	0.62212	4.58703	3.27070
H	-2.84631	-2.44354	3.71497
H	1.07536	-4.12791	4.37757
H	2.94424	-1.52207	2.65441
H	3.03499	-2.98435	3.68260
H	2.89646	-1.37489	4.42006
H	-2.55068	-4.52600	5.10344
H	-0.93288	-5.25684	5.29290
H	-1.81357	-5.42258	3.75878
H	-1.82553	0.88946	3.33256
H	-3.13515	-0.24875	2.90510
H	-1.92223	0.23754	1.68851
H	-0.13787	-4.20412	-3.47959
H	2.61229	-3.77874	-3.15456
H	6.03287	-0.24158	-2.27766
H	5.38611	-2.83096	1.11795
H	1.89640	-3.07928	0.94886
H	3.35579	-4.01982	1.38358
H	2.47559	-4.36113	-0.13005
H	7.94838	-0.97395	-0.87802
H	7.69629	-2.08017	0.50075
H	7.31547	-0.35228	0.66159
H	3.31211	-1.21150	-4.16211
H	4.31695	0.22251	-3.83006
H	2.62890	0.13337	-3.23342
H	-4.50260	-2.24115	-3.80830

H -4.03643 -4.01341 0.10243
H -0.54216 -4.43352 -0.04451
H -1.91830 -4.28742 1.08777
H -0.82245 -2.90269 0.80937
H -6.33859 -3.72336 -2.74931
H -6.47529 -2.45476 -1.51490
H -6.19869 -4.14201 -1.01843
H -1.23167 -0.80119 -4.03864
H -2.70210 -1.26596 -4.94496
H -1.30164 -2.36476 -4.87682
H -1.41281 5.26457 -0.33180
H -3.52874 6.25295 0.55842
H -5.50457 4.80929 1.04556
H -4.35045 -0.86309 -0.49733
H -6.43710 0.11258 0.47297
H -6.57827 2.54419 1.00935

TS(1-4)_gas
SCF = -2554.88006346
H(0 K)= -2553.943065
H(298 K)= -2553.879452
G(298 K)= -2554.042047
SCF(D3BJ) = -2555.22274273
SCF(BS2) = -4338.45143589
SCF(BS2+D3BJ) = -4338.79411510
Low Freq. = -67.3794cm-1, 11.5966cm-1

Ni 0.45365 -0.12981 -0.20106
N 2.21791 -2.63991 -0.42165
N 0.15161 -3.14079 -0.80161
N 1.46169 2.35882 0.90290
N -0.27411 1.67882 2.04227
C 0.95369 -2.05329 -0.45444
C 2.18769 -4.00509 -0.72831
H 3.09294 -4.60558 -0.75385
C 0.88656 -4.31954 -0.96768
H 0.40676 -5.25749 -1.23424
C 3.50367 -2.03040 -0.16359
C 4.11608 -2.26188 1.08861
C 5.45199 -1.84989 1.25754
H 5.93963 -2.02947 2.22362
C 6.17942 -1.24634 0.21794
C 5.52827 -1.02667 -1.01117
H 6.07861 -0.55531 -1.83423
C 4.19551 -1.41267 -1.23335
C 3.38713 -2.97627 2.20584
H 3.33603 -4.06599 2.02615
H 2.34892 -2.62176 2.30559
H 3.90278 -2.82373 3.16742
C 7.63555 -0.87184 0.39905
H 7.93564 -0.90910 1.45901
H 7.84327 0.14362 0.02004
H 8.29694 -1.56193 -0.15628
C 3.54322 -1.21855 -2.58153
H 3.18640 -2.17891 -2.99486
H 4.25477 -0.78021 -3.29895
H 2.65949 -0.56024 -2.51559
C -1.28248 -3.20102 -0.98535
C -2.09848 -3.42652 0.14769
C -3.47163 -3.65558 -0.06173
H -4.11356 -3.83459 0.80906
C -4.03314 -3.68318 -1.35187
C -3.18241 -3.47526 -2.45321
H -3.60018 -3.50372 -3.46649
C -1.80248 -3.24530 -2.30394
C -1.50651 -3.45681 1.53600
H -1.05479 -2.48430 1.79174
H -0.70988 -4.21817 1.61481
H -2.27931 -3.68380 2.28634
C -5.51562 -3.90870 -1.55590
H -5.98322 -4.36477 -0.66809
H -5.70897 -4.56350 -2.42235
H -6.03175 -2.95095 -1.75140
C -0.91646 -3.07409 -3.51505
H -0.10238 -3.82008 -3.53393
H -0.44717 -2.07434 -3.51423
H -1.50301 -3.18361 -4.44079
C 0.53419 1.30149 0.96037
C 0.13157 2.89704 2.60000
H -0.38934 3.33631 3.44595
C 1.21509 3.31859 1.89538
H 1.84588 4.19700 2.00382
C 2.73987 2.39497 0.21649
C 2.88472 3.05443 -1.02622
C 4.18282 3.21032 -1.54770
H 4.29947 3.72787 -2.50777
C 5.32465 2.75614 -0.86680
C 5.14383 2.11886 0.37271
H 6.01982 1.77086 0.93187
C 3.86946 1.92569 0.93270
C 1.70858 3.60795 -1.79267
H 1.14678 2.78787 -2.27681
H 2.04593 4.29543 -2.58463
H 1.02444 4.16753 -1.13046
C 6.70630 2.94172 -1.45734
H 7.48181 2.96567 -0.67345
H 6.77752 3.87771 -2.03643
H 6.96156 2.11587 -2.14737
C 3.71786 1.26328 2.28305
H 3.30083 1.95930 3.03329
H 4.69019 0.90095 2.65017
H 3.03024 0.40325 2.22267
C -1.33447 0.91900 2.66511
C -2.65068 1.43942 2.67254
C -3.64327 0.71873 3.36464
H -4.66859 1.10756 3.35471
C -3.36100 -0.46573 4.06390
C -2.02943 -0.92065 4.08022
H -1.77493 -1.82026 4.65425
C -1.00047 -0.24510 3.40154
C -3.00774 2.75600 2.02104

H	-2.33003	3.00446	1.19320
H	-2.96159	3.58298	2.75516
H	-4.03408	2.72908	1.62382
C	-4.45658	-1.23338	4.77296
H	-5.23139	-0.55793	5.17254
H	-4.05705	-1.82946	5.61043
H	-4.96343	-1.93395	4.08368
C	0.42639	-0.72851	3.50037
H	0.82043	-0.97926	2.49721
H	0.49602	-1.61458	4.15191
H	1.08691	0.05476	3.91361
Cl	0.07672	0.29114	-2.71320
C	-6.07390	0.43165	-0.88627
H	-6.95172	-0.20574	-0.72633
C	-6.24656	1.77118	-1.21359
H	-7.24927	2.19832	-1.32255
C	-5.11123	2.61501	-1.40285
C	-4.09359	4.78623	-1.87133
H	-4.19435	5.84959	-2.11732
C	-5.23049	4.00244	-1.71768
H	-6.22970	4.43583	-1.83349
H	-1.91382	4.88193	-1.81755
C	-2.79824	4.24355	-1.70802
C	-2.63664	2.88530	-1.39533
C	-3.79427	2.04756	-1.25848
C	-3.64222	0.65119	-0.95722
C	-4.78583	-0.13593	-0.75446
H	-4.66487	-1.19282	-0.49968
N	-1.38396	2.32484	-1.15644
H	-0.60112	2.95354	-1.31227
B	-1.13529	0.89152	-1.03302
N	-2.35467	0.11388	-0.89423
H	-2.30972	-0.90123	-0.80574

Int(1-4)2_gas

SCF = -2554.89505613
H(0 K)= -2553.957153
H(298 K)= -2553.893195
G(298 K)= -2554.057344
SCF(D3BJ) = -2555.23084779
SCF(BS2) = -4338.45652026
SCF(BS2+D3BJ) = -4338.80162967
Low Freq. = 7.4241cm-1, 15.5335cm-1

Ni	0.36371	0.04542	-0.40438
N	2.45556	-2.32503	-0.85258
N	0.39575	-2.85978	-1.21947
N	1.28037	2.08739	1.35445
N	-0.47076	1.17599	2.29330
C	1.17093	-1.80418	-0.73659
C	2.46413	-3.62318	-1.38151
H	3.39002	-4.16880	-1.54290
C	1.16647	-3.95843	-1.61040
H	0.71389	-4.86377	-2.00620
C	3.73540	-1.74043	-0.50783
C	4.32510	-2.10625	0.72387
C	5.65947	-1.72509	0.95940
H	6.12995	-2.01350	1.90750
C	6.41078	-1.02210	0.00026
C	5.78813	-0.68448	-1.21570
H	6.36342	-0.15455	-1.98468
C	4.45580	-1.03638	-1.50114
C	3.57631	-2.94467	1.73620
H	3.44993	-3.98405	1.38186
H	2.56388	-2.55100	1.92224
H	4.11887	-2.98072	2.69403
C	7.84945	-0.63493	0.27080
H	8.31429	-1.30022	1.01688
H	7.92088	0.39694	0.66236
H	8.45683	-0.67203	-0.64904
C	3.84435	-0.73263	-2.84727
H	3.61288	-1.66375	-3.39650
H	4.53698	-0.13776	-3.46348
H	2.89144	-0.18297	-2.74840
C	-1.04625	-2.94667	-1.32539
C	-1.77689	-3.41365	-0.20844
C	-3.16445	-3.61232	-0.35601
H	-3.73784	-3.97255	0.50659
C	-3.81852	-3.40168	-1.58358
C	-3.04567	-2.98487	-2.68385
H	-3.53156	-2.83921	-3.65587
C	-1.65918	-2.76545	-2.59158
C	-1.08197	-3.78812	1.07954
H	-0.33128	-3.03755	1.36681
H	-0.55360	-4.75366	0.97042
H	-1.80703	-3.88948	1.90095
C	-5.30793	-3.62634	-1.73175
H	-5.73318	-4.12561	-0.84602
H	-5.53409	-4.24626	-2.61642
H	-5.83780	-2.66636	-1.86677
C	-0.86082	-2.40070	-3.81935
H	-0.09273	-3.16341	-4.04045
H	-0.33620	-1.43908	-3.67547
H	-1.52120	-2.31655	-4.69687
C	0.35546	1.04027	1.16681
C	-0.07977	2.24949	3.10481
H	-0.61386	2.49568	4.01823
C	1.01018	2.81272	2.52190
H	1.63475	3.64913	2.82444
C	2.56940	2.28545	0.71468
C	2.72012	3.17031	-0.37664
C	4.02467	3.44826	-0.82975
H	4.14623	4.13606	-1.67527
C	5.16451	2.90250	-0.21851
C	4.97699	2.04696	0.88258
H	5.84980	1.62302	1.39186
C	3.69851	1.72414	1.36508
C	1.54849	3.83734	-1.05317
H	1.08435	3.13300	-1.76998
H	1.87592	4.72522	-1.61718
H	0.79050	4.15830	-0.31831

C 6.55300 3.21913 -0.72980
H 7.27460 3.32687 0.09794
H 6.56546 4.14967 -1.32041
H 6.92709 2.40942 -1.38281
C 3.54381 0.84160 2.58284
H 3.14766 1.40628 3.44630
H 4.51288 0.40686 2.87077
H 2.83974 0.01570 2.39031
C -1.53492 0.30581 2.74071
C -2.86301 0.79278 2.77174
C -3.86156 -0.04651 3.30262
H -4.89610 0.31664 3.31251
C -3.57110 -1.31704 3.82935
C -2.22808 -1.73928 3.83615
H -1.96987 -2.70591 4.28604
C -1.19409 -0.94444 3.31009
C -3.22197 2.19004 2.32024
H -2.54045 2.56363 1.54227
H -3.17676 2.89867 3.16866
H -4.24857 2.21777 1.92404
C -4.67078 -2.20569 4.37071
H -5.49955 -1.61224 4.79091
H -4.29599 -2.88037 5.15832
H -5.09924 -2.84069 3.57334
C 0.24802 -1.38134 3.41907
H 0.74445 -1.35336 2.43299
H 0.32120 -2.40026 3.83090
H 0.81681 -0.70457 4.08252
Cl 0.46209 0.62179 -2.64343
C -6.19716 0.48873 -0.80714
H -7.06889 -0.16202 -0.67130
C -6.37595 1.80262 -1.22398
H -7.37836 2.19557 -1.42537
C -5.24958 2.66481 -1.38842
C -4.24800 4.82727 -1.93160
H -4.35508 5.86973 -2.25244
C -5.37615 4.02576 -1.80051
H -6.37414 4.42511 -2.01094
H -2.07791 4.97919 -1.74901
C -2.95449 4.32892 -1.65142
C -2.78713 2.99855 -1.24094
C -3.93270 2.14237 -1.11982
C -3.77407 0.77250 -0.71835
C -4.90787 -0.03521 -0.55169
H -4.78073 -1.07179 -0.22551
N -1.53323 2.47412 -0.91889
H -0.74848 3.09076 -1.11401
B -1.28276 1.08809 -0.60521
N -2.48115 0.29077 -0.48783
H -2.42259 -0.69991 -0.25030

4_gas

SCF = -2554.92378405
H(0 K)= -2553.984696
H(298 K)= -2553.920934
G(298 K)= -2554.084663
SCF(D3BJ) = -2555.26784704
SCF(BS2) = -4338.49272200
SCF(BS2+D3BJ) = -4338.83704575
Low Freq. = 10.2852cm-1, 15.1115cm-1

Ni 0.00003 -0.96784 0.00002
Cl 0.00006 -3.30931 0.00008
N 0.98382 -0.88585 -2.80561
N -1.16424 -1.18587 -2.74563
N -0.98377 -0.88575 2.80565
N 1.16430 -1.18572 2.74568
N -1.20207 1.76645 0.10144
H -2.10538 1.30874 0.22087
N 1.20198 1.76652 -0.10154
H 2.10533 1.30887 -0.22095
C -0.07812 -0.94565 -1.91103
C 0.57127 -1.10665 -4.12344
H 1.27799 -1.10805 -4.94866
C -0.77668 -1.29339 -4.08547
H -1.50007 -1.48946 -4.87221
C -2.57151 -1.23546 -2.39841
C -3.30908 -0.02661 -2.43104
C -4.69090 -0.08788 -2.17299
H -5.27047 0.84325 -2.19601
C -5.34921 -1.30711 -1.93107
C -4.59237 -2.49024 -1.98316
H -5.09567 -3.45568 -1.85019
C -3.20641 -2.48972 -2.23334
C -2.45850 -3.79149 -2.38373
H -2.01484 -3.88259 -3.39187
H -3.13753 -4.64624 -2.23462
H -1.62833 -3.86050 -1.65768
C -6.83441 -1.34566 -1.64078
H -7.03215 -1.21852 -0.56043
H -7.28115 -2.30731 -1.94328
H -7.37143 -0.53791 -2.16610
C -2.66860 1.28191 -2.83758
H -1.70734 1.44633 -2.32878
H -3.32608 2.13347 -2.60205
H -2.47535 1.29975 -3.92625
C 2.35282 -0.50372 -2.52849
C 2.73143 0.83501 -2.79792
C 4.07805 1.19258 -2.59709
H 4.38024 2.22790 -2.79607
C 5.04102 0.25799 -2.17460
C 4.63212 -1.07189 -1.97126
H 5.37419 -1.82466 -1.68001
C 3.29839 -1.48646 -2.15247
C 2.91798 -2.93884 -2.00809
H 2.12988 -3.08598 -1.24797
H 3.79637 -3.54327 -1.73162
H 2.51356 -3.33755 -2.95625
C 6.47802 0.67643 -1.94733
H 6.76622 1.51223 -2.60656

H	7.17557	-0.15831	-2.12908
H	6.63483	1.01389	-0.90618
C	1.75112	1.85230	-3.33975
H	1.60901	1.72677	-4.42898
H	2.11606	2.87574	-3.16239
H	0.76247	1.75948	-2.86583
C	0.07817	-0.94556	1.91107
C	-0.57122	-1.10649	4.12348
H	-1.27794	-1.10788	4.94870
C	0.77673	-1.29320	4.08553
H	1.50013	-1.48922	4.87227
C	2.57156	-1.23527	2.39846
C	3.20651	-2.48953	2.23347
C	4.59246	-2.49002	1.98327
H	5.09581	-3.45545	1.85035
C	5.34927	-1.30687	1.93112
C	4.69092	-0.08764	2.17298
H	5.27046	0.84351	2.19595
C	3.30910	-0.02640	2.43103
C	2.66858	1.28212	2.83749
H	1.70731	1.44649	2.32870
H	3.32603	2.13369	2.60191
H	2.47534	1.30002	3.92617
C	6.83447	-1.34539	1.64083
H	7.28130	-2.30689	1.94366
H	7.37142	-0.53741	2.16586
H	7.03219	-1.21862	0.56043
C	2.45864	-3.79131	2.38391
H	2.01498	-3.88238	3.39206
H	3.13770	-4.64605	2.23484
H	1.62847	-3.86038	1.65787
C	-2.35278	-0.50365	2.52850
C	-3.29832	-1.48643	2.15250
C	-4.63206	-1.07190	1.97128
H	-5.37411	-1.82469	1.68004
C	-5.04099	0.25798	2.17459
C	-4.07804	1.19260	2.59705
H	-4.38027	2.22792	2.79600
C	-2.73142	0.83508	2.79789
C	-1.75113	1.85240	3.33968
H	-1.60898	1.72687	4.42891
H	-2.11613	2.87582	3.16234
H	-0.76250	1.75962	2.86573
C	-6.47800	0.67637	1.94732
H	-7.17553	-0.15841	2.12895
H	-6.63480	1.01395	0.90620
H	-6.76627	1.51209	2.60663
C	-2.91787	-2.93880	2.00814
H	-2.12974	-3.08593	1.24804
H	-3.79623	-3.54325	1.73165
H	-2.51346	-3.33750	2.95631
C	-1.24150	3.16414	0.10184
C	-2.44608	3.87523	0.19878
H	-3.38945	3.32387	0.27850
C	-2.43604	5.29024	0.19786
H	-3.38856	5.82688	0.27463
C	-1.24849	6.00452	0.10138
H	-1.25296	7.09969	0.10147
C	-0.00016	5.31966	-0.00009
C	-0.00011	3.87838	-0.00008
C	1.24132	3.16422	-0.10197
C	2.44585	3.87538	-0.19893
H	3.38926	3.32408	-0.27864
C	2.43572	5.29039	-0.19804
H	3.38821	5.82709	-0.27482
C	1.24813	6.00460	-0.10157
H	1.25253	7.09976	-0.10169
B	-0.00002	0.96394	-0.00003

TS(1-4)

SCF = -2540.37258572
H(0 K)= -2539.432595
H(298 K)= -2539.369559
G(298 K)= -2539.535633
SCF(D3BJ) = -2540.64829559
SCF(BS2) = -3878.66721182
SCF(BS2+D3BJ) = -3878.99453049
Low Freq. = -418.0182cm-1, 3.7169cm-1

Ni	-0.17305	0.64615	-0.01736
N	-0.62017	1.67046	-2.76408
N	1.34374	0.75480	-2.64382
N	-1.37891	0.33687	2.71307
N	0.50641	1.40933	2.79804
C	0.24690	1.08045	-1.83996
C	-0.08098	1.70141	-4.05354
H	-0.62000	2.13636	-4.89121
C	1.15278	1.12545	-3.97898
H	1.91258	0.95515	-4.73721
C	-1.90246	2.26839	-2.47977
C	-1.94797	3.60433	-2.02198
C	-3.21134	4.19231	-1.82648
H	-3.25992	5.22674	-1.46434
C	-4.40595	3.49725	-2.09339
C	-4.31542	2.17255	-2.56122
H	-5.23495	1.61193	-2.76978
C	-3.07738	1.53722	-2.76502
C	-0.67791	4.38198	-1.76239
H	-0.08522	4.50526	-2.68695
H	-0.03357	3.85293	-1.03877
H	-0.90514	5.38463	-1.36696
C	-5.75189	4.16951	-1.91854
H	-6.07411	4.66792	-2.85187
H	-5.71957	4.94198	-1.13248
H	-6.53622	3.44141	-1.65299
C	-3.00036	0.11110	-3.25797
H	-2.56408	0.04863	-4.27123
H	-4.00144	-0.34716	-3.29229
H	-2.35723	-0.48861	-2.59085
C	2.57260	0.14452	-2.20436
C	3.52296	0.93452	-1.51777
C	4.73782	0.32881	-1.14556
H	5.47973	0.92995	-0.60616
C	5.03085	-1.01153	-1.46168

C	4.06492	-1.75756	-2.16367
H	4.26820	-2.80613	-2.41034
C	2.82959	-1.20329	-2.54867
C	3.24993	2.38675	-1.20759
H	2.44263	2.48627	-0.46023
H	2.92165	2.93234	-2.10961
H	4.15083	2.87776	-0.80944
C	6.36586	-1.62448	-1.09222
H	6.78651	-1.16437	-0.18269
H	7.10664	-1.48252	-1.90098
H	6.27884	-2.71020	-0.92057
C	1.81195	-2.03362	-3.29806
H	1.76367	-1.75628	-4.36692
H	0.80137	-1.89454	-2.88023
H	2.06601	-3.10310	-3.23866
C	-0.36386	0.81496	1.87926
C	0.04589	1.30316	4.11550
H	0.59595	1.72185	4.95435
C	-1.13669	0.62785	4.05884
H	-1.83119	0.33191	4.84072
C	-2.56613	-0.38970	2.32734
C	-2.59642	-1.78870	2.52853
C	-3.79142	-2.47210	2.23273
H	-3.82400	-3.55865	2.37652
C	-4.93594	-1.80121	1.76296
C	-4.87013	-0.40408	1.60192
H	-5.75793	0.13986	1.25657
C	-3.70071	0.32608	1.88136
C	-1.39425	-2.53321	3.06518
H	-1.54089	-3.62085	2.98070
H	-1.21094	-2.29664	4.12929
H	-0.47961	-2.26504	2.51116
C	-6.20162	-2.56348	1.42901
H	-6.20680	-2.88749	0.37176
H	-7.09984	-1.94216	1.58209
H	-6.30152	-3.47137	2.04669
C	-3.66039	1.82445	1.70625
H	-3.26469	2.32944	2.60478
H	-4.66524	2.22347	1.49601
H	-2.99345	2.08197	0.86348
C	1.69868	2.15812	2.48713
C	2.95585	1.52303	2.58486
C	4.10908	2.31171	2.40255
H	5.09231	1.83191	2.48073
C	4.03482	3.69092	2.13862
C	2.76065	4.28679	2.05088
H	2.68211	5.36303	1.85355
C	1.57976	3.54496	2.22666
C	3.06264	0.05108	2.91442
H	2.32551	-0.54122	2.34739
H	2.86409	-0.13748	3.98544
H	4.07214	-0.32833	2.69079
C	5.28833	4.51720	1.93886
H	6.18568	3.98150	2.28857
H	5.22963	5.47675	2.48073
H	5.44250	4.76159	0.87166
C	0.22236	4.20843	2.17469
H	-0.43841	3.69888	1.45167
H	0.31312	5.26776	1.88738
H	-0.28362	4.16193	3.15601
H	-1.68927	0.50993	-0.29470
C	-2.02851	-5.79544	-0.73074
H	-2.92789	-6.38632	-0.93987
C	-0.81516	-6.43985	-0.51619
H	-0.74705	-7.53250	-0.55439
C	0.36412	-5.68334	-0.24092
C	2.75281	-5.51305	0.25245
H	3.72286	-5.99317	0.42639
C	1.63453	-6.29473	-0.01323
H	1.71119	-7.38686	-0.05080
H	3.55782	-3.50025	0.52272
C	2.66839	-4.10219	0.30783
C	1.43898	-3.46077	0.09175
C	0.26847	-4.24524	-0.19070
C	-0.99704	-3.60331	-0.42374
C	-2.13212	-4.38595	-0.68767
H	-3.09506	-3.89319	-0.85985
N	1.30546	-2.06979	0.14659
H	2.18028	-1.56125	0.26741
B	0.07340	-1.33603	-0.09118
N	-1.04486	-2.21091	-0.37971
H	-1.96523	-1.78339	-0.48631

TS(1-9)

SCF = -2540.40069379
H(0 K)= -2539.457660
H(298 K)= -2539.395887
G(298 K)= -2539.554069
SCF(D3BJ) = -2540.73452195
SCF(BS2) = -3878.74299320
SCF(BS2+D3BJ) = -3879.07682137
Low Freq. = -183.3268cm-1, 15.8925cm-1

Ni	0.77580	-0.32954	-0.42243
N	-0.28854	0.35047	2.30837
N	1.03476	1.90151	1.48129
N	0.91341	-3.11181	-1.13405
N	2.90657	-2.48758	-0.51187
C	0.18387	0.83740	1.07359
C	0.31634	1.00009	3.38417
H	0.09813	0.72248	4.41234
C	1.14105	1.95623	2.87023
H	1.79055	2.67610	3.36147
C	-1.37980	-0.57175	2.55825
C	-1.09539	-1.91857	2.87237
C	-2.17154	-2.76081	3.21375
H	-1.95845	-3.80651	3.46651
C	-3.49767	-2.29672	3.25692
C	-3.73280	-0.93515	2.98647
H	-4.75405	-0.54165	3.04974
C	-2.69203	-0.04694	2.66234
C	0.32370	-2.42984	2.89688
H	0.92349	-1.90706	3.66375
H	0.82009	-2.25343	1.92602
H	0.35060	-3.50613	3.13023
C	-4.64288	-3.22908	3.59055
H	-5.19213	-3.52712	2.67869
H	-5.37418	-2.74715	4.26143
H	-4.28547	-4.15112	4.07767
C	-2.97110	1.42970	2.51197

H	-2.49705	1.84750	1.61132
H	-2.58100	1.99090	3.38133
H	-4.05295	1.61768	2.44303
C	1.52115	3.01535	0.68972
C	2.60530	2.84922	-0.20255
C	3.04724	3.97208	-0.93191
H	3.88017	3.83981	-1.63284
C	2.46814	5.24170	-0.78017
C	1.40630	5.37588	0.13611
H	0.93289	6.35589	0.27104
C	0.91704	4.28941	0.88378
C	3.27315	1.51977	-0.37843
H	2.53313	0.74469	-0.71983
H	3.68953	1.13695	0.56856
H	4.08553	1.57441	-1.11795
C	2.98093	6.43743	-1.55358
H	3.56250	6.12784	-2.43683
H	3.64027	7.06503	-0.92595
H	2.15318	7.08147	-1.89539
C	-0.25011	4.49946	1.82439
H	0.05316	4.45013	2.88468
H	-1.02556	3.73181	1.66896
H	-0.70688	5.48649	1.65251
C	1.59369	-1.99148	-0.61591
C	3.00599	-3.81904	-0.94107
H	3.95170	-4.35473	-0.92360
C	1.75974	-4.20904	-1.32608
H	1.39411	-5.15422	-1.71871
C	-0.45772	-3.13627	-1.58556
C	-0.79730	-2.49553	-2.80730
C	-2.12694	-2.58324	-3.25202
H	-2.39948	-2.08181	-4.18833
C	-3.11083	-3.30322	-2.54569
C	-2.72492	-3.96769	-1.36941
H	-3.46617	-4.55892	-0.81783
C	-1.40519	-3.91143	-0.87650
C	0.23505	-1.76460	-3.63197
H	0.58197	-0.85719	-3.10147
H	-0.18415	-1.46649	-4.60603
H	1.12494	-2.39357	-3.81060
C	-4.53867	-3.34853	-3.04512
H	-5.12236	-4.13253	-2.53559
H	-4.58058	-3.53986	-4.13124
H	-5.04331	-2.38177	-2.86653
C	-1.02322	-4.71736	0.34489
H	-0.67353	-5.72798	0.06108
H	-1.88902	-4.84531	1.01311
H	-0.21052	-4.24019	0.91104
C	4.11116	-1.74137	-0.23181
C	4.86070	-1.25310	-1.33140
C	6.09242	-0.62560	-1.07330
H	6.67935	-0.25041	-1.92077
C	6.59064	-0.47062	0.23422
C	5.82172	-0.97301	1.29871
H	6.19885	-0.87880	2.32452
C	4.58475	-1.61572	1.09319
C	4.35011	-1.39398	-2.74765
H	4.27600	-2.45284	-3.05318
H	5.01782	-0.88039	-3.45715
H	3.33784	-0.96427	-2.84429
C	7.90789	0.23183	0.48699
H	8.36520	-0.09657	1.43470
H	7.76908	1.32682	0.55237
H	8.62876	0.04500	-0.32637
C	3.80462	-2.14509	2.27292
H	3.00392	-1.44063	2.55735
H	4.46155	-2.28146	3.14714
H	3.31730	-3.10672	2.04531
H	0.06772	0.70167	-1.47569
C	-5.77270	0.31268	-0.95790
H	-6.62295	-0.37995	-0.93869
C	-5.99224	1.66626	-1.19241
H	-7.00365	2.05095	-1.36328
C	-4.89167	2.57636	-1.21337
C	-3.95743	4.81886	-1.47636
H	-4.09516	5.88908	-1.67174
C	-5.06175	3.97344	-1.45712
H	-6.07032	4.36321	-1.63340
H	-1.79277	5.01253	-1.26867
C	-2.65126	4.33113	-1.24789
C	-2.43653	2.96349	-0.99291
C	-3.56304	2.06725	-0.98475
C	-3.35751	0.66003	-0.75379
C	-4.47330	-0.19916	-0.73999
H	-4.31864	-1.26772	-0.55522
N	-1.16768	2.45931	-0.75566
H	-0.41617	3.13129	-0.90146
B	-0.82740	1.01752	-0.54847
N	-2.07416	0.19352	-0.54146
H	-1.99166	-0.82025	-0.46390

Int(1-9)1

SCF = -2540.40415293
H(0 K)= -2539.460924
H(298 K)= -2539.398437
G(298 K)= -2539.559453
SCF(D3BJ) = -2540.73438839
SCF(BS2) = -3878.74653910
SCF(BS2+D3BJ) = -3879.07677453
Low Freq. = 11.7093cm-1, 18.5720cm-1

Ni	0.68744	-0.39855	-0.50569
N	-0.05486	0.26370	2.33340
N	1.33927	1.71854	1.40898
N	0.60958	-3.20388	-1.19178
N	2.65085	-2.70022	-0.63418
C	0.21191	0.91170	1.10928
C	0.93392	0.56390	3.27314
H	0.92580	0.12265	4.26624
C	1.78939	1.46121	2.70267
H	2.67712	1.94830	3.09810
C	-1.25757	-0.44069	2.73054
C	-1.19160	-1.83016	2.98350
C	-2.36045	-2.48137	3.42617
H	-2.31600	-3.55965	3.62210
C	-3.56698	-1.79241	3.63236
C	-3.57645	-0.39963	3.42388
H	-4.49531	0.16657	3.61688
C	-2.43733	0.30283	2.99452
C	0.09595	-2.60346	2.82912

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H    0.83020 -2.32879  3.60798
H    0.56804 -2.40050  1.85172
H   -0.08790 -3.68502  2.92289
C   -4.82056 -2.51802  4.07180
H   -5.53967 -2.60864  3.23745
H   -5.33791 -1.97651  4.88233
H   -4.59495 -3.53600  4.42894
C   -2.47756  1.80643  2.87127
H   -2.38136  2.12639  1.82043
H   -1.65064  2.27181  3.43552
H   -3.42665  2.20144  3.26556
C    1.81365  2.88593  0.68747
C    2.75835  2.74457 -0.35530
C    3.20718  3.91220 -1.00612
H    3.92993  3.80630 -1.82405
C    2.77402  5.19399 -0.63131
C    1.86115  5.29807  0.43726
H    1.51435  6.28869  0.75525
C    1.36752  4.16750  1.11181
C    3.28427  1.39767 -0.75249
H    2.43915  0.68537 -0.96343
H    3.87437  0.93248  0.05562
H    3.92095  1.46698 -1.64783
C    3.26094  6.43113 -1.35504
H    4.13604  6.21113 -1.98736
H    3.54045  7.22930 -0.64606
H    2.47280  6.84450 -2.01034
C    0.35156  4.33255  2.21858
H    0.66878  3.84014  3.15388
H   -0.60952  3.87888  1.91968
H    0.17908  5.39881  2.43231
C    1.37046 -2.13624 -0.69480
C    2.66281 -4.03121 -1.06832
H    3.57621 -4.62028 -1.08354
C    1.38304 -4.34600 -1.41753
H    0.95205 -5.26523 -1.80516
C   -0.78303 -3.14532 -1.57938
C   -1.14136 -2.42766 -2.75269
C   -2.48900 -2.43461 -3.14418
H   -2.77578 -1.87208 -4.04043
C   -3.47672 -3.14253 -2.43019
C   -3.07615 -3.87591 -1.30246
H   -3.82300 -4.45296 -0.74321
C   -1.73647 -3.90366 -0.86212
C   -0.11479 -1.68562 -3.57347
H    0.27016 -0.81511 -3.00329
H   -0.55457 -1.32585 -4.51710
H    0.75426 -2.32443 -3.81029
C   -4.92332 -3.09721 -2.87106
H   -5.53558 -3.83949 -2.33349
H   -5.02203 -3.28957 -3.95357
H   -5.35325 -2.09774 -2.67915
C   -1.36536 -4.77054  0.32177
H   -1.27864 -5.83235  0.02478
H   -2.14290 -4.71582  1.10143
H   -0.40599 -4.47328  0.76736
C    3.89540 -2.00985 -0.38072
C    4.64594 -1.56668 -1.49807
C    5.90707 -0.99014 -1.26490
H    6.49631 -0.64956 -2.12505
C    6.43065 -0.84115  0.03319
C    5.65567 -1.29500  1.11548
H    6.05116 -1.20344  2.13455
C    4.38985 -1.88710  0.93622
C    4.10746 -1.69813 -2.90515
H    3.97334 -2.75455 -3.19788
H    4.79040 -1.22848 -3.63023
H    3.11848 -1.21542 -2.99294
C    7.78110 -0.19448  0.25809
H    8.25091 -0.55344  1.18852
H    7.68740  0.90402  0.34142
H    8.47101 -0.39861 -0.57744
C    3.60047 -2.36199  2.13250
H    2.84033 -1.61247  2.41523
H    4.26175 -2.51831  3.00014
H    3.06429 -3.30208  1.92575
H   -0.02070  0.79422 -1.26650
C   -5.68463  0.58918 -1.12088
H   -6.56480 -0.06568 -1.12277
C   -5.79678  1.89565 -1.58586
H   -6.75189  2.27999 -1.96053
C   -4.65895  2.75871 -1.57334
C   -3.59205  4.91396 -1.99967
H   -3.64737  5.94781 -2.36156
C   -4.72508  4.10809 -2.03631
H   -5.67695  4.49297 -2.41861
H   -1.48133  5.08648 -1.47330
C   -2.36093  4.43230 -1.50173
C   -2.24903  3.11192 -1.02484
C   -3.40473  2.25314 -1.07438
C   -3.30666  0.89074 -0.61358
C   -4.45798  0.07870 -0.64041
H   -4.38773 -0.95595 -0.28694
N   -1.06880  2.63610 -0.47829
H   -0.27681  3.26429 -0.60966
B   -0.78808  1.16893 -0.19089
N   -2.09993  0.42372 -0.13286
H   -2.08592 -0.57518  0.07049
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SCF  =       -1964.91313676
H(0 K)=      -1964.204126
H(298 K)=    -1964.159216
G(298 K)=    -1964.279878
SCF(D3BJ) = -1965.15872847
SCF(BS2) = -1965.58085008
SCF(BS2+D3BJ) = -
1965.82644180
Low Freq. = 16.1395cm-1,
20.9418cm-1

N  -2.49539  1.92134  0.43947
N  -0.46341  2.62814  0.71510
N   0.19747 -0.65862  0.07270
N  -1.54355 -0.29443 -1.68914
H  -1.78180  0.06077 -2.61261
N   2.52101 -0.09160 -0.76723
H   2.19195  0.81366 -1.10197
N   2.19325 -2.23043  0.33357
H   1.61217 -2.94103  0.77897
C  -1.19028  1.61184  0.14023
C  -2.57330  3.09789  1.18850
```

H	-3.52833	3.49776	1.51773
C	-1.29420	3.54167	1.36314
H	-0.89443	4.41134	1.87736
C	0.97410	2.80841	0.67017
C	1.75527	2.30812	1.73531
C	3.13661	2.57049	1.70816
H	3.75970	2.18311	2.52238
C	3.73846	3.30448	0.66940
C	2.91662	3.79636	-0.36324
H	3.36439	4.38397	-1.17357
C	1.52798	3.56817	-0.38548
C	0.66805	4.11904	-1.50091
H	0.19504	3.30268	-2.07513
H	1.27235	4.72134	-2.19665
H	-0.14592	4.75749	-1.11489
C	5.23395	3.52742	0.64479
H	5.73452	2.68508	0.13312
H	5.65158	3.58923	1.66305
H	5.49860	4.45071	0.10372
C	1.13397	1.51686	2.86306
H	0.37222	2.10381	3.40644
H	1.90187	1.20450	3.58732
H	0.63367	0.61326	2.47357
C	-3.70090	1.19976	0.07342
C	-4.25480	0.29385	1.00422
C	-5.46866	-0.32753	0.65780
H	-5.91150	-1.03869	1.36445
C	-6.12215	-0.06654	-0.55924
C	-5.54582	0.86742	-1.44055
H	-6.05176	1.10015	-2.38523
C	-4.33794	1.52295	-1.14429
C	-3.75923	2.54869	-2.09337
H	-3.68225	3.54512	-1.62254
H	-4.38927	2.64784	-2.99086
H	-2.74175	2.27027	-2.41742
C	-7.39803	-0.79356	-0.92248
H	-7.16686	-1.77458	-1.37651
H	-7.99855	-0.22494	-1.65131
H	-8.02225	-0.98618	-0.03413
C	-3.59419	0.01092	2.33498
H	-2.62694	-0.50429	2.20379
H	-4.23628	-0.63484	2.95321
H	-3.39855	0.93893	2.90090
C	-0.66605	-1.62374	0.66050
C	-0.37833	-2.20853	1.90551
H	0.48587	-1.84995	2.47428
C	-1.18280	-3.25743	2.42166
H	-0.93019	-3.69355	3.39490
C	-2.26731	-3.73919	1.70382
H	-2.86655	-4.57246	2.08802
C	-2.61626	-3.16598	0.44200
C	-1.83766	-2.05723	-0.05695
C	-2.20271	-1.43751	-1.31170
C	-3.22770	-2.02136	-2.08184
H	-3.48510	-1.57725	-3.05035
C	-3.95237	-3.13007	-1.59709
H	-4.75257	-3.55050	-2.21778
C	-3.68548	-3.68233	-0.34719
H	-4.26780	-4.52843	0.03300
C	3.85944	-0.38393	-1.00928
C	4.70530	0.50945	-1.68507
H	4.30396	1.46610	-2.03663
C	6.06075	0.17317	-1.91206
H	6.69987	0.88505	-2.44716
C	6.58916	-1.03636	-1.47658
H	7.63972	-1.28702	-1.65883
C	5.76336	-1.97674	-0.78895
C	4.38018	-1.64443	-0.55467
C	3.52557	-2.57907	0.12530
C	4.04726	-3.80807	0.55532
H	3.39310	-4.52138	1.06909
C	5.40612	-4.12345	0.32319
H	5.79070	-5.09005	0.66805
C	6.25358	-3.23693	-0.33081
H	7.30379	-3.49305	-0.50747
B	-0.51574	0.40448	-0.80725
H	0.27822	1.02307	-1.51008
B	1.59821	-0.98244	-0.09996

H2

SCF = -1.17652777705
H(0 K)= -1.166622
H(298 K)= -1.163317
G(298 K)= -1.178130
SCF(D3BJ) = -1.17663781617
SCF(BS2) = -1.17765460100
SCF(BS2+D3BJ) = -1.17776464356
Low Freq. = 4348.1357cm-1, cm-1

H	0.00000	0.00000	0.37552
H	0.00000	0.00000	-0.37552

[Ni(IMes)]$_2$

SCF = -2190.57172732
H(0 K)= -2189.798890
H(298 K)= -2189.745331
G(298 K)= -2189.884825
SCF(D3BJ) = -2190.82888656
SCF(BS2) = -4866.28757543
SCF(BS2+D3BJ) = -4866.54473475
Low Freq. = 20.4260cm-1, 24.2261cm-1

N	-3.41803	-1.72150	0.11485
N	-1.30241	-2.19186	0.04583
C	-2.16890	-1.09144	0.01343
C	-1.98565	-3.41079	0.15873
H	-1.46245	-4.36306	0.19305
C	-3.31584	-3.11545	0.20269
H	-4.19058	-3.75587	0.28626
C	-4.68597	-1.03977	0.11734
C	-5.26398	-0.66159	1.35031
C	-6.53712	-0.06064	1.32898
H	-6.99540	0.23787	2.28007
C	-7.23614	0.16046	0.12708
C	-5.35057	-0.82307	-1.11181
Ni	-1.81816	0.70602	-0.09279
C	-2.31467	2.47933	1.03515

```
C  -2.96025  2.56668 -0.23346
C  -2.16408  2.39108 -1.40326
H  -2.64623  2.41734 -2.38679
C  -0.75174  2.19367 -1.33686
C  -0.13374  2.16693 -0.04731
C   0.75192 -2.19453 -1.33558
H   2.64642 -2.41939 -2.38525
H  -2.91341  2.56925  1.94845
C  -0.90719  2.27332  1.15278
C   0.13388 -2.16658 -0.04607
Ni  1.81784 -0.70585 -0.09272
C   2.16425 -2.39219 -1.40177
C   2.96033 -2.56693 -0.23181
C   2.31474 -2.47834  1.03670
H   2.91346 -2.56750  1.95009
C   0.90729 -2.27205  1.15414
N   3.41812  1.72159  0.11372
N   1.30254  2.19215  0.04462
C   2.16891  1.09163  0.01260
C   1.98591  3.41105  0.15703
H   1.46281  4.36340  0.19087
C   3.31607  3.11559  0.20106
H   4.19089  3.75595  0.28425
C   4.68597  1.03970  0.11661
C   5.35009  0.82132 -1.11251
C   6.62121  0.21922 -1.08159
H   7.14519  0.04409 -2.02954
C   7.23599 -0.16083  0.12696
C   6.53746  0.06191  1.32882
H   6.99607 -0.23542  2.28012
C   5.26440  0.66308  1.34985
C  -6.62175 -0.22105 -1.08120
H  -7.14608 -0.04717 -2.02919
C  -8.62336  0.76855  0.13362
H  -8.79284  1.39903 -0.75526
H  -9.40356 -0.01523  0.12816
H  -8.78983  1.38770  1.03046
C  -4.52710 -0.88639  2.65100
H  -3.55019 -0.37156  2.63364
H  -5.11156 -0.51018  3.50576
H  -4.31869 -1.95735  2.82160
C  -4.70123 -1.21815 -2.41855
H  -4.51214 -2.30525 -2.46658
H  -5.33717 -0.94210 -3.27473
H  -3.72059 -0.72081 -2.52726
C   4.43927 -2.86205 -0.32903
H   4.85224 -2.51905 -1.29073
H   4.99902 -2.35841  0.47548
H   4.63272 -3.94881 -0.24802
C   8.62313 -0.76911  0.13378
H   8.78952 -1.38788  1.03090
H   8.79255 -1.39998 -0.75483
H   9.40340  0.01459  0.12799
C   0.24394 -2.21610  2.51204
H   0.98700 -1.99356  3.29470
H  -0.53632 -1.43863  2.53512
H  -0.23839 -3.17831  2.76863
C  -0.07479 -2.08628 -2.59654
H  -0.58485 -3.04169 -2.82375
H  -0.85208 -1.31150 -2.49128
H   0.56510 -1.83304 -3.45720
C  -4.43926  2.86131 -0.33107
H  -4.99881  2.35893  0.47436
H  -4.63298  3.94816 -0.25196
H  -4.85220  2.51650 -1.29214
C   0.07501  2.08433 -2.59770
H  -0.56505  1.83162 -3.45839
H   0.58616  3.03912 -2.82501
H   0.85143  1.30871 -2.49218
C  -0.24391  2.21859  2.51076
H   0.23832  3.18106  2.76658
H  -0.98699  1.99663  3.29356
H   0.53641  1.44121  2.53454
C   4.52818  0.88992  2.65056
H   4.32072  1.96125  2.82003
H   3.55085  0.37590  2.63423
H   5.11267  0.51425  3.50554
C   4.70031  1.21482 -2.41950
H   4.51115  2.30184 -2.46874
H   5.33596  0.93778 -3.27557
H   3.71965  0.71729 -2.52722
```

Bdan_rad

```
SCF  =       -520.264728518
H(0 K)=      -520.105300
H(298 K)=    -520.095224
G(298 K)=    -520.139801
SCF(D3BJ) = -520.309969775
SCF(BS2) = -520.450036095
SCF(BS2+D3BJ) = -
520.495277353
Low Freq. = 125.8422cm-1,
157.2474cm-1

C  -2.44523 -1.38430  0.00026
H  -3.39927 -1.92246  0.00054
C  -1.25122 -2.09241  0.00014
H  -1.25135 -3.18744  0.00016
C   0.00010 -1.40465  0.00000
C   2.44544 -1.38395 -0.00031
H   3.39955 -1.92196 -0.00051
C   1.25154 -2.09224 -0.00011
H   1.25185 -3.18726 -0.00000
H   3.40787  0.57752 -0.00015
C   2.45769  0.03194 -0.00017
C   1.25342  0.74077  0.00012
C   0.00001  0.03743 -0.00005
C  -1.25349  0.74055 -0.00017
C  -2.45768  0.03157  0.00019
H  -3.40792  0.57704  0.00026
N   1.21799  2.14967  0.00075
H   2.12585  2.61143  0.00124
B  -0.00024  2.87990  0.00007
N  -1.21835  2.14952 -0.00071
H  -2.12632  2.61106 -0.00156
```

Int(1-3)4

```
SCF  =       -2034.57747185
H(0 K)=      -2033.801655
H(298 K)=    -2033.747431
G(298 K)=    -2033.894893
SCF(D3BJ) = -2034.83228556
```

SCF(BS2) = -3817.96438161
SCF(BS2+D3BJ) = -
3818.21919532
Low Freq. = 7.0899cm-1,
17.1602cm-1

Ni	0.00078	-0.00278	-0.20725
N	0.56028	-2.79746	0.62118
N	-1.41300	-2.67010	-0.25649
N	1.43965	2.64727	-0.30160
N	-0.53132	2.81293	0.57334
C	-0.32174	-1.88051	0.07170
C	0.03915	-4.09528	0.62855
H	0.60152	-4.94165	1.01412
C	-1.20589	-4.01292	0.07531
H	-1.96236	-4.77165	-0.10724
C	1.87556	-2.49600	1.13615
C	2.04065	-2.36620	2.53559
C	3.34348	-2.17732	3.02955
H	3.48733	-2.08024	4.11272
C	4.46126	-2.11940	2.17460
C	4.24995	-2.24543	0.78958
H	5.10867	-2.20293	0.10936
C	2.96692	-2.43564	0.24099
C	0.85479	-2.42925	3.47350
H	0.36879	-3.42085	3.45595
H	0.08227	-1.69385	3.18866
H	1.16536	-2.22277	4.50987
C	5.85200	-1.90797	2.73596
H	6.00746	-2.48934	3.66066
H	6.02420	-0.84608	2.99198
H	6.62898	-2.20209	2.01174
C	2.76503	-2.56881	-1.25017
H	2.21655	-3.49287	-1.50392
H	3.73288	-2.58569	-1.77513
H	2.16724	-1.72650	-1.64473
C	-2.66608	-2.22018	-0.82194
C	-3.62129	-1.62786	0.03225
C	-4.86586	-1.26988	-0.52020
H	-5.61669	-0.80941	0.13311
C	-5.17318	-1.49720	-1.87307
C	-4.19834	-2.10931	-2.68367
H	-4.42093	-2.30238	-3.74027
C	-2.93768	-2.48219	-2.18581
C	-3.32907	-1.38905	1.49570
H	-2.58797	-0.57966	1.62168
H	-2.91298	-2.28966	1.98014
H	-4.24527	-1.09880	2.03339
C	-6.51226	-1.08905	-2.45069
H	-7.24177	-0.85881	-1.65714
H	-6.93809	-1.88425	-3.08666
H	-6.41497	-0.18885	-3.08465
C	-1.90399	-3.10870	-3.09167
H	-1.51238	-4.05838	-2.68791
H	-1.05138	-2.41424	-3.20426
H	-2.33017	-3.30817	-4.08789
C	0.34286	1.87553	0.04842
C	-0.00049	4.10644	0.54425
H	-0.55501	4.96618	0.91112
C	1.24330	4.00039	-0.00812
H	2.00463	4.74854	-0.21282
C	2.67952	2.17006	-0.87338
C	2.91664	2.36750	-2.25397
C	4.16358	1.96643	-2.76600
H	4.36026	2.10949	-3.83556
C	5.15761	1.39162	-1.95183
C	4.88534	1.23147	-0.58135
H	5.65312	0.80369	0.07443
C	3.65541	1.61719	-0.01562
C	1.86315	2.96661	-3.15530
H	0.97326	2.31028	-3.17061
H	2.24450	3.06867	-4.18382
H	1.53812	3.96341	-2.80882
C	6.47887	0.94567	-2.54238
H	7.26076	0.86337	-1.76955
H	6.83361	1.64693	-3.31662
H	6.38513	-0.04494	-3.02424
C	3.39756	1.44857	1.46400
H	2.99612	2.37245	1.91555
H	4.32530	1.17951	1.99274
H	2.65786	0.64890	1.64608
C	-1.84635	2.53715	1.10495
C	-2.95471	2.53370	0.22883
C	-4.23290	2.36839	0.79724
H	-5.10477	2.36886	0.13242
C	-4.42293	2.21315	2.18220
C	-3.28870	2.21720	3.01759
H	-3.41599	2.09946	4.10081
C	-1.99026	2.37989	2.50377
C	-2.77742	2.69924	-1.26188
H	-2.20251	3.61049	-1.50335
H	-3.75465	2.76391	-1.76565
H	-2.21739	1.84710	-1.69019
C	-5.80932	2.03022	2.76426
H	-6.59062	2.34152	2.05202
H	-5.93864	2.61412	3.69151
H	-5.99987	0.97208	3.02237
C	-0.78548	2.39004	3.41883
H	-0.04849	1.62684	3.11329
H	-1.08326	2.18886	4.45999
H	-0.26226	3.36253	3.39631
Cl	-0.18581	0.03508	-2.55077

Int(1-4)3
SCF = -2020.06411994
H(0 K)= -2019.284683
H(298 K)= -2019.231581
G(298 K)= -2019.375684
SCF(D3BJ) = -2020.30894567
SCF(BS2) = -3358.22825463
SCF(BS2+D3BJ) = -
3358.47308039
Low Freq. = 13.5894cm-1,
21.6336cm-1

Ni	0.00092	0.00079	-0.19128
N	-0.71563	2.78236	0.47504
N	1.25211	2.67169	-0.43134
N	-1.25186	-2.66616	-0.45691
N	0.71590	-2.78779	0.44782
C	0.20988	1.85505	-0.00059
C	-0.26256	4.10018	0.33776

```
H  -0.86127  4.95237  0.64921
C   0.97574  4.02940 -0.23279
H   1.68157  4.80708 -0.51329
C  -1.98079  2.44884  1.07963
C  -2.07883  2.44244  2.49056
C  -3.33743  2.18717  3.06417
H  -3.42712  2.18116  4.15756
C  -4.47817  1.94383  2.27568
C  -4.33561  1.95153  0.87562
H  -5.21178  1.76038  0.24465
C  -3.09813  2.19815  0.25209
C  -0.86346  2.69130  3.35585
H  -0.47767  3.71980  3.23851
H  -0.04030  2.00946  3.07915
H  -1.10239  2.53810  4.42022
C  -5.81823  1.65637  2.92108
H  -5.94695  2.22615  3.85665
H  -5.91760  0.58559  3.17874
H  -6.65380  1.90921  2.24770
C  -2.96078  2.18135 -1.25229
H  -2.51753  3.11972 -1.62969
H  -3.94036  2.04030 -1.73519
H  -2.28810  1.36105 -1.56666
C   2.48123  2.21210 -1.02910
C   3.57274  1.89105 -0.19285
C   4.78654  1.52428 -0.80470
H   5.64290  1.27473 -0.16655
C   4.92993  1.47343 -2.20343
C   3.81310  1.78974 -3.00091
H   3.90113  1.74423 -4.09349
C   2.58003  2.16614 -2.43930
C   3.43529  1.92146  1.31218
H   2.72603  1.14520  1.65101
H   3.04440  2.89095  1.66714
H   4.40651  1.74057  1.79906
C   6.25817  1.11777 -2.83918
H   6.91105  0.57433 -2.13661
H   6.80377  2.02484 -3.15935
H   6.12229  0.49081 -3.73663
C   1.38399  2.47863 -3.30710
H   0.99621  3.49624 -3.12313
H   0.56748  1.76879 -3.07583
H   1.63949  2.39444 -4.37543
C  -0.20897 -1.85491 -0.01774
C   0.26182 -4.10377  0.29693
H   0.85986 -4.95954  0.59973
C  -0.97650 -4.02609 -0.27268
H  -1.68297 -4.80026 -0.56117
C  -2.48024 -2.19893 -1.05021
C  -2.58033 -2.14353 -2.45947
C  -3.81560 -1.76704 -3.01748
H  -3.90714 -1.72024 -4.10966
C  -4.93098 -1.45575 -2.21709
C  -4.78857 -1.52339 -0.81846
H  -5.64807 -1.29023 -0.17822
C  -3.57340 -1.89016 -0.21053
C  -1.38654 -2.45401 -3.33106
H  -0.56738 -1.74880 -3.09536
H  -1.64293 -2.36053 -4.39840
H  -1.00191 -3.47433 -3.15563
C  -6.24453 -1.03744 -2.84519
H  -7.10099 -1.29033 -2.19823
H  -6.39818 -1.52290 -3.82345
H  -6.27674  0.05445 -3.01735
C  -3.43715 -1.94118  1.29408
H  -3.04098 -2.91313  1.63616
H  -4.40973 -1.77214  1.78252
H  -2.73257 -1.16558  1.64411
C   1.98045 -2.46160  1.05767
C   3.10005 -2.20637  0.23460
C   4.33677 -1.96826  0.86299
H   5.21471 -1.77380  0.23551
C   4.47626 -1.97284  2.26339
C   3.33316 -2.21965  3.04736
H   3.42040 -2.22287  4.14096
C   2.07526 -2.46700  2.46878
C   2.96608 -2.17571 -1.26992
H   2.52827 -3.11257 -1.65745
H   3.94589 -2.02465 -1.74914
H   2.29024 -1.35555 -1.57770
C   5.81569 -1.69426  2.91404
H   6.65208 -1.94580  2.24116
H   5.93999 -2.27051  3.84622
H   5.91828 -0.62550  3.17877
C   0.85710 -2.72041  3.32877
H   0.03391 -2.03922  3.05063
H   1.09169 -2.57001  4.39450
H   0.47366 -3.74932  3.20696
H  -0.00168  0.00754 -1.72687
```

10

```
SCF  =       -2019.94804556
H(0 K)=      -2019.165225
H(298 K)=    -2019.111847
G(298 K)=    -2019.258259
SCF(D3BJ) = -2020.18697658
SCF(BS2) = -3358.10563087
SCF(BS2+D3BJ) = -
3358.34456189
Low Freq. = 9.0352cm-1,
16.3127cm-1

Ni  0.03654  0.04551  0.02057
N   0.59235  0.28031  2.83617
N  -1.01384 -1.14871  2.53970
N   0.97861 -0.36037 -2.72373
N  -0.56907  1.15906 -2.63917
C  -0.16599 -0.31200  1.85021
C   0.22751 -0.17296  4.10424
H   0.71475  0.18353  5.00788
C  -0.78522 -1.07429  3.91613
H  -1.35862 -1.66539  4.62509
C  -2.01395 -2.00697  1.94028
C  -1.64736 -3.31931  1.56493
C  -2.64973 -4.14468  1.02254
H  -2.38730 -5.16827  0.73068
C  -3.97467 -3.69955  0.85536
C  -4.29445 -2.38657  1.25266
H  -5.32413 -2.02677  1.14129
C  -3.33329 -1.51845  1.80047
C  -3.70219 -0.11427  2.22357
H  -3.48794  0.06087  3.29232
```

H	-4.77413	0.07308	2.05823
H	-3.12962	0.63854	1.65369
C	-5.02722	-4.60190	0.24832
H	-5.14037	-4.40564	-0.83369
H	-6.01440	-4.43941	0.71149
H	-4.76296	-5.66532	0.36289
C	-0.23189	-3.82290	1.73640
H	0.47176	-3.26481	1.09316
H	-0.16323	-4.88939	1.47217
H	0.12134	-3.70607	2.77551
C	1.62605	1.25451	2.55587
C	2.95853	0.80831	2.39540
C	3.94474	1.78129	2.14670
H	4.98430	1.45517	2.02630
C	3.63755	3.15251	2.06189
C	2.29711	3.55041	2.23629
H	2.04249	4.61564	2.19011
C	1.26992	2.62301	2.48680
C	-0.15779	3.07768	2.69736
H	-0.84250	2.62206	1.96077
H	-0.23533	4.17170	2.60562
H	-0.52927	2.79349	3.69761
C	4.71622	4.17516	1.77812
H	5.71686	3.78668	2.02597
H	4.55336	5.10188	2.35264
H	4.72576	4.45479	0.70879
C	3.31993	-0.65643	2.50863
H	3.14732	-1.03723	3.53087
H	4.38148	-0.81440	2.26537
H	2.71398	-1.27855	1.82787
C	0.16396	0.31198	-1.83932
C	0.76423	0.06531	-4.03425
H	1.32109	-0.34595	-4.87204
C	-0.21276	1.02411	-3.98079
H	-0.67875	1.61861	-4.76213
C	-1.56586	2.09145	-2.15371
C	-2.90992	1.66485	-2.05695
C	-3.85785	2.60057	-1.60464
H	-4.90551	2.28770	-1.52341
C	-3.50340	3.92102	-1.26701
C	-2.15312	4.30096	-1.38478
H	-1.85992	5.32602	-1.12967
C	-1.16224	3.40662	-1.83002
C	0.28011	3.84576	-1.95777
H	0.94569	3.25166	-1.30684
H	0.39071	4.90501	-1.67955
H	0.65361	3.72634	-2.98973
C	-4.55459	4.91550	-0.82424
H	-5.05654	5.37198	-1.69686
H	-4.11407	5.73503	-0.23403
H	-5.33786	4.43350	-0.21642
C	-3.32031	0.25458	-2.41636
H	-2.97764	-0.02744	-3.42678
H	-4.41552	0.14870	-2.38589
H	-2.88686	-0.47861	-1.71264
C	1.94942	-1.36543	-2.34089
C	1.53881	-2.71576	-2.26375
C	2.50859	-3.67087	-1.90809
H	2.20836	-4.72331	-1.84277
C	3.84670	-3.31723	-1.64787
C	4.20943	-1.96038	-1.74389
H	5.24747	-1.66693	-1.54862
C	3.28107	-0.96214	-2.09269
C	3.70310	0.48694	-2.20099
H	3.54567	0.88254	-3.21966
H	4.77029	0.60042	-1.95651
H	3.12667	1.13250	-1.51540
C	4.87597	-4.37389	-1.30994
H	5.30125	-4.81674	-2.22910
H	4.43413	-5.19884	-0.72745
H	5.71435	-3.95247	-0.73226
C	0.11121	-3.12536	-2.54741
H	-0.58065	-2.71137	-1.79224
H	0.01197	-4.22155	-2.53749
H	-0.23083	-2.76125	-3.53161
H	-1.02853	-0.84533	-0.24117

ClBdan$^-$

SCF = -534.891114274
H(0 K)= -534.743163
H(298 K)= -534.731726
G(298 K)= -534.779440
SCF(D3BJ) = -534.938638389
SCF(BS2) = -980.312253046
SCF(BS2+D3BJ) = -980.359777161
Low Freq. = 79.0835cm-1, 136.2221cm-1

C	-2.81498	1.29053	0.00002
C	-2.15429	0.01987	-0.00001
C	-0.70940	-0.01442	0.00003
C	0.01580	1.22534	0.00001
C	-0.66665	2.45565	0.00005
C	-2.08009	2.47108	0.00004
C	0.02009	-1.27967	0.00029
C	-0.76238	-2.46597	0.00004
C	-2.16844	-2.42362	-0.00007
C	-2.86777	-1.21433	-0.00002
N	1.39469	-1.35027	-0.00004
B	2.06171	-0.14001	-0.00046
N	1.40844	1.15066	-0.00014
H	-2.72981	-3.36786	-0.00016
H	-3.96416	-1.19672	-0.00004
H	-2.60109	3.43691	0.00004
H	-3.91146	1.31587	0.00002
H	-0.09534	3.39192	0.00004
H	-0.22433	-3.42035	-0.00001
H	1.90860	2.03913	-0.00018
Cl	3.93034	-0.02873	0.00010

HBdan$^-$

SCF = -520.398038058
H(0 K)= -520.242749
H(298 K)= -520.232683
G(298 K)= -520.276625
SCF(D3BJ) = -520.442113793
SCF(BS2) = -520.593278090
SCF(BS2+D3BJ) = -520.637353842
Low Freq. = 126.2007cm-1, 148.5154cm-1

```
C   2.41448 -0.52071 -0.00034
C   2.69027  0.85664 -0.00019
C   1.66858  1.81268  0.00013
C   0.30561  1.39547  0.00016
C   0.01357 -0.02121  0.00006
C   1.07909 -1.02223  0.00001
C  -1.35683 -0.45201 -0.00014
C  -2.40428  0.49306 -0.00012
C  -2.10155  1.87283  0.00003
C  -0.78519  2.32470  0.00017
N  -1.58771 -1.82186 -0.00030
B  -0.49435 -2.79309  0.00028
N   0.84615 -2.37301  0.00043
H   3.73717  1.19161 -0.00036
H   1.89892  2.88513  0.00040
H  -2.92544  2.59854  0.00000
H  -0.56433  3.39939  0.00022
H  -3.44550  0.14663 -0.00025
H   3.22144 -1.26195 -0.00075
H  -2.57037 -2.09777 -0.00088
H  -0.83186 -3.96731  0.00061
```

Int(1-2)1

```
SCF  =       -2440.99387588
H(0 K)=      -2440.126780
H(298 K)=    -2440.065711
G(298 K)=    -2440.223922
SCF(D3BJ) = -2441.30129421
SCF(BS2) = -4224.53541463
SCF(BS2+D3BJ) = -
4224.84283301
Low Freq. = 14.1512cm-1,
21.7817cm-1

Ni  0.25249 -0.14182  0.00376
N   0.82857 -2.36530 -1.78907
N  -1.27193 -1.89267 -2.02900
N   1.76456  1.69225  1.87226
N   0.09466  0.66863  2.80774
C  -0.13911 -1.46596 -1.33874
C   0.31556 -3.29117 -2.69978
H   0.93578 -4.06680 -3.14108
C  -1.00357 -2.99242 -2.85118
H  -1.78288 -3.46165 -3.44529
C   2.18893 -2.51559 -1.31917
C   2.42536 -3.40090 -0.23965
C   3.76000 -3.67029  0.11396
H   3.95619 -4.35587  0.94727
C   4.84260 -3.10454 -0.58535
C   4.56319 -2.24830 -1.66677
H   5.39346 -1.81426 -2.23689
C   3.24692 -1.94417 -2.06338
C   1.28190 -4.08220  0.47960
H   0.76242 -4.79787 -0.18335
H   0.52256 -3.35673  0.81735
H   1.64785 -4.63913  1.35628
C   6.27009 -3.39990 -0.17600
H   6.35980 -4.39610  0.28793
H   6.63417 -2.66306  0.56410
H   6.95519 -3.35812 -1.03881
C   2.97857 -1.07140 -3.26592
H   2.41612 -1.61995 -4.04269
H   3.92333 -0.72247 -3.71156
H   2.37314 -0.19071 -2.99058
C  -2.64781 -1.45660 -1.91319
C  -3.37854 -1.80370 -0.75634
C  -4.75530 -1.50896 -0.73358
H  -5.33186 -1.77211  0.16149
C  -5.41079 -0.91879 -1.82786
C  -4.64825 -0.61382 -2.97156
H  -5.14123 -0.16087 -3.84086
C  -3.26516 -0.86148 -3.03835
C  -2.72274 -2.50262  0.40998
H  -1.98587 -1.84445  0.90467
H  -2.17903 -3.40638  0.08156
H  -3.47303 -2.80182  1.15755
C  -6.88840 -0.59520 -1.77060
H  -7.42011 -1.25250 -1.06283
H  -7.36528 -0.69678 -2.75996
H  -7.05135  0.44600 -1.43619
C  -2.47041 -0.45523 -4.25873
H  -1.94791 -1.30419 -4.73180
H  -1.70395  0.28356 -3.96818
H  -3.12805  0.00186 -5.01516
C   0.74685  0.78522  1.58312
C   0.67675  1.46904  3.79404
H   0.29628  1.49504  4.81168
C   1.72479  2.11146  3.20431
H   2.45467  2.80923  3.60561
C   2.86627  2.08661  1.01777
C   2.95826  3.42331  0.56432
C   4.07549  3.77252 -0.21579
H   4.15035  4.80187 -0.58707
C   5.08840  2.85048 -0.53462
C   4.98498  1.54794 -0.01515
H   5.78241  0.82227 -0.21568
C   3.89216  1.14589  0.77376
C   1.91522  4.46247  0.90581
H   0.90278  4.07595  0.71011
H   2.07044  5.37236  0.30438
H   1.96374  4.75608  1.97071
C   6.25288  3.24931 -1.41620
H   7.14410  2.63180 -1.21507
H   6.52728  4.30771 -1.27148
H   6.00043  3.12296 -2.48522
C   3.84290 -0.24177  1.36605
H   3.55498 -0.21480  2.43147
H   4.82379 -0.73472  1.28411
H   3.10337 -0.87359  0.84387
C  -0.96004 -0.26278  3.14513
C  -2.29882  0.18558  3.18535
C  -3.28095 -0.71820  3.63522
H  -4.32444 -0.38244  3.66780
C  -2.96316 -2.02254  4.05299
C  -1.61277 -2.42255  4.01899
H  -1.34043 -3.42919  4.35930
C  -0.59294 -1.55970  3.58104
C  -2.66557  1.59820  2.79879
H  -2.39448  2.31305  3.59785
H  -3.74857  1.68934  2.62384
H  -2.13516  1.91808  1.88978
```

```
C  -4.04261 -2.97886  4.51482
H  -4.94843 -2.44003  4.83718
H  -3.69660 -3.60410  5.35519
H  -4.34104 -3.66751  3.70270
C   0.85591 -1.99016  3.62076
H   1.34276 -1.87105  2.63795
H   0.94317 -3.04410  3.92801
H   1.43533 -1.37862  4.33594
C  -2.53796  4.33467  0.17187
C  -3.82562  4.63219 -0.32914
H  -4.35869  5.50900  0.05322
C  -4.42688  3.82455 -1.31037
H  -5.42405  4.08043 -1.68401
C  -3.76815  2.68801 -1.83213
H  -4.23055  2.04996 -2.58901
H  -2.05887  4.95723  0.93343
C  -1.89192  3.21445 -0.35410
C  -2.49513  2.40084 -1.33668
O  -1.65062  1.37850 -1.68248
O  -0.65559  2.71966 -0.03415
B  -0.42830  1.55240 -0.90282
Cl  1.08107  1.85199 -2.06502
```

TS(1-2)

```
SCF  =       -2440.98223000
H(0 K)=      -2440.115352
H(298 K)=    -2440.054625
G(298 K)=    -2440.213058
SCF(D3BJ) = -2441.29001027
SCF(BS2) = -4224.52165243
SCF(BS2+D3BJ) = -
4224.82943272
Low Freq. = -70.9169cm-1,
16.0195cm-1

Ni  0.29283 -0.12232  0.01250
N   1.07539 -2.55053 -1.39314
N  -1.04048 -2.30565 -1.77573
N   1.74004  2.04470  1.42633
N   0.08710  1.23713  2.58839
C   0.00914 -1.71125 -1.09260
C   0.70147 -3.60440 -2.22927
H   1.41404 -4.35450 -2.56150
C  -0.62942 -3.44749 -2.47141
H  -1.32877 -4.03765 -3.05704
C   2.40555 -2.51402 -0.82304
C   2.64780 -3.28850  0.33862
C   3.97061 -3.37710  0.80860
H   4.17334 -3.97787  1.70347
C   5.03697 -2.74039  0.14571
C   4.75267 -1.99162 -1.01105
H   5.57270 -1.50013 -1.54754
C   3.44725 -1.86409 -1.52473
C   1.53346 -4.05278  1.02059
H   1.17929 -4.88817  0.38957
H   0.65757 -3.41216  1.21785
H   1.87892 -4.47662  1.97644
C   6.45162 -2.84770  0.67452
H   6.61365 -3.80019  1.20572
H   6.67323 -2.03499  1.39148
H   7.19335 -2.77504 -0.13781
C   3.18164 -1.09951 -2.79784
H   2.78365 -1.76464 -3.58556
H   4.10925 -0.64138 -3.17470
H   2.42830 -0.30297 -2.65105
C  -2.45264 -1.98159 -1.76073
C  -3.21336 -2.31882 -0.61958
C  -4.60419 -2.12008 -0.67578
H  -5.20774 -2.38020  0.20235
C  -5.23940 -1.62025 -1.82800
C  -4.44185 -1.30693 -2.94415
H  -4.91764 -0.91732 -3.85239
C  -3.04366 -1.47203 -2.93769
C  -2.56584 -2.88494  0.62274
H  -1.91679 -2.13523  1.10908
H  -1.93215 -3.75881  0.38805
H  -3.33002 -3.20078  1.35033
C  -6.73960 -1.41155 -1.85648
H  -7.26999 -2.21517 -1.31787
H  -7.12365 -1.37879 -2.88917
H  -7.02033 -0.45872 -1.37059
C  -2.21368 -1.07990 -4.13795
H  -1.65488 -1.93441 -4.55885
H  -1.46781 -0.31280 -3.85722
H  -2.85597 -0.67105 -4.93410
C   0.73130  1.09310  1.36523
C   0.66990  2.24069  3.36281
H   0.29907  2.48945  4.35339
C   1.70798  2.74562  2.63379
H   2.43535  3.52035  2.86115
C   2.85915  2.20912  0.51497
C   2.87592  3.28010 -0.40801
C   4.03544  3.44726 -1.18872
H   4.05992  4.27058 -1.91245
C   5.15540  2.60692 -1.06497
C   5.11008  1.57804 -0.10725
H   5.98460  0.93132  0.03142
C   3.97779  1.36227  0.69858
C   1.70862  4.21855 -0.58272
H   0.90928  3.71561 -1.15187
H   2.02081  5.12235 -1.13001
H   1.27187  4.52370  0.38230
C   6.37336  2.80288 -1.94254
H   7.28373  2.39870 -1.46952
H   6.54443  3.86948 -2.16470
H   6.24891  2.28706 -2.91238
C   3.98022  0.27170  1.74511
H   3.61121  0.63744  2.71891
H   4.99853 -0.12087  1.89077
H   3.33818 -0.57544  1.44650
C  -0.97547  0.39859  3.10249
C  -2.29008  0.90838  3.18524
C  -3.28174  0.08019  3.74839
H  -4.30837  0.46154  3.80578
C  -2.99471 -1.20226  4.24364
C  -1.66096 -1.65357  4.18515
H  -1.40728 -2.63787  4.59719
C  -0.63411 -0.87201  3.62964
C  -2.63915  2.31180  2.74586
H  -2.58254  3.01371  3.59897
H  -3.66857  2.35521  2.35682
H  -1.95875  2.68019  1.96619
```

```
C  -4.08569 -2.08026  4.81856
H  -4.93771 -1.48193  5.18025
H  -3.71311 -2.69216  5.65712
H  -4.47669 -2.77909  4.05615
C   0.79641 -1.36008  3.64555
H   1.20392 -1.46076  2.62478
H   0.86808 -2.33887  4.14499
H   1.45511 -0.65324  4.18093
C  -2.71418  4.38632 -0.57166
C  -4.04659  4.57809 -1.00058
H  -4.47547  5.58516 -0.97453
C  -4.82809  3.50246 -1.46111
H  -5.85676  3.68555 -1.78877
C  -4.31299  2.18794 -1.51465
H  -4.90622  1.34254 -1.87284
H  -2.09920  5.21578 -0.21097
C  -2.21443  3.08632 -0.63457
C  -2.99541  2.01063 -1.09523
O  -2.25646  0.84806 -1.03865
O  -0.97309  2.62003 -0.25502
B  -0.95531  1.22412 -0.60118
Cl  0.39824  1.30123 -2.72596
```

Int(1-2)2

```
SCF  =       -2440.99318175
H(0 K)=      -2440.124250
H(298 K)=    -2440.062949
G(298 K)=    -2440.226224
SCF(D3BJ) = -2441.29620021
SCF(BS2) = -4224.52456619
SCF(BS2+D3BJ) = -
4224.82758465
Low Freq. = 1.3843cm-1,
17.7777cm-1

C   2.54211 -1.68522 -1.97727
C   1.74639 -0.72567 -2.64134
C   2.28436  0.47452 -3.16207
C   3.65237  0.71825 -2.94815
C   4.47686 -0.18394 -2.24828
C   3.90287 -1.38671 -1.79234
N   0.33641 -0.99851 -2.83397
C  -0.63637 -0.91422 -1.85813
N  -1.79919 -1.24215 -2.52969
C  -1.55205 -1.53046 -3.87161
C  -0.20614 -1.37462 -4.06064
C  -3.11993 -1.29274 -1.94095
C  -3.90870 -0.11957 -1.94241
C  -5.21985 -0.21873 -1.43996
C  -5.74532 -1.42983 -0.95180
C  -4.92259 -2.57307 -0.97191
C  -3.60771 -2.53463 -1.46986
Ni -0.53717 -0.57042 -0.00130
B   0.39391  1.04286 -0.25092
O   1.70892  1.27854  0.17561
C   2.00257  2.58569 -0.22097
C   0.87324  3.13530 -0.84702
C   0.86043  4.44137 -1.33238
C   2.05147  5.18013 -1.16087
C   3.18328  4.61802 -0.53685
C   3.18879  3.29387 -0.04670
O  -0.14762  2.18107 -0.88599
C  -3.37149  1.18849 -2.47685
C  -7.15499 -1.50427 -0.40542
C  -2.76623 -3.79115 -1.53573
C   1.43803  1.46572 -3.93298
C   5.92206  0.14438 -1.96483
C   1.96329 -2.98968 -1.47814
C  -0.44158 -0.29314  1.86158
N   0.27866 -1.07883  2.73928
C   0.11211 -0.65640  4.05657
C  -0.72312  0.42579  4.01985
N  -1.05038  0.63767  2.68153
C   1.06906 -2.24210  2.38885
C   2.47649 -2.11459  2.32586
C   3.21693 -3.28619  2.07580
C   2.60402 -4.54060  1.89895
C   1.20003 -4.61756  1.97880
C   0.40776 -3.48288  2.23124
C  -1.94134  1.69626  2.25546
C  -1.46868  3.02915  2.26819
C  -2.37002  4.04073  1.88909
C  -3.69900  3.76044  1.52159
C  -4.13171  2.42155  1.55206
C  -3.27412  1.36859  1.91961
C   3.16724 -0.78620  2.52284
C   3.43337 -5.77507  1.61634
C  -1.09547 -3.60429  2.36836
C  -0.06128  3.37972  2.69874
C  -4.63396  4.87132  1.09339
C  -3.77803 -0.05597  1.96769
Cl  6.25365  2.00733  1.41371
H  -0.02341  4.86466 -1.81766
H   2.09296  6.21191 -1.52499
H   4.09086  5.21933 -0.42535
H   4.07704  2.85230  0.43376
H   0.59667 -1.16338  4.88664
H  -1.11697  1.05538  4.81282
H   4.30918 -3.20893  2.02844
H   0.70615 -5.58967  1.86197
H   2.86615 -0.05897  1.75057
H   4.25979 -0.89604  2.46781
H   2.92164 -0.33780  3.50133
H   3.59901 -5.90275  0.53062
H   2.93579 -6.68918  1.97978
H   4.42650 -5.70984  2.08981
H  -1.44219 -3.24750  3.35439
H  -1.41212 -4.65293  2.25715
H  -1.63431 -3.00632  1.61101
H  -2.01822  5.07908  1.88585
H  -5.17145  2.18654  1.29541
H   0.68361  2.66097  2.32305
H   0.03172  3.39181  3.80012
H   0.21691  4.37976  2.33389
H  -4.44480  5.79896  1.65848
H  -5.68994  4.58975  1.23661
H  -4.49898  5.11145  0.02280
H  -3.42546 -0.58379  2.86985
H  -3.43235 -0.63383  1.09142
H  -4.87865 -0.07717  1.96301
H   0.41316 -1.50262 -4.94409
H  -2.34730 -1.81682 -4.55463
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H  -5.85000  0.67830 -1.44092
H  -5.31837 -3.52800 -0.60582
H  -2.49814  1.53441 -1.89734
H  -4.14449  1.97098 -2.43617
H  -3.04139  1.08913 -3.52604
H  -7.15386 -1.51070  0.69993
H  -7.66488 -2.42640 -0.73111
H  -7.76055 -0.64330 -0.73064
H  -2.63929 -4.13582 -2.57779
H  -3.24028 -4.60760 -0.96957
H  -1.75231 -3.63247 -1.13091
H   4.08314  1.65268 -3.32536
H   4.53329 -2.11402 -1.26786
H   1.21746  1.10830 -4.95566
H   1.96421  2.42800 -4.02399
H   0.47210  1.65232 -3.43577
H   6.53727 -0.76788 -1.89144
H   6.01343  0.68407 -0.99901
H   6.35025  0.79351 -2.74655
H   1.40039 -2.84622 -0.53765
H   2.76689 -3.71296 -1.27134
H   1.27178 -3.44066 -2.21068
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2

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SCF  =       -2441.02321134
H(0 K)=      -2440.155383
H(298 K)=    -2440.094186
G(298 K)=    -2440.254833
SCF(D3BJ) = -2441.33402074
SCF(BS2) = -4224.56500357
SCF(BS2+D3BJ) = -
4224.87581302
Low Freq. = 12.5521cm-1,
16.1907cm-1

C   2.62970 -3.05165 -2.34821
C   2.52821 -1.64338 -2.21855
C   3.63153 -0.85190 -1.82877
C   4.82488 -1.51343 -1.47662
C   4.94967 -2.91177 -1.53135
C   3.84605 -3.65691 -1.98679
N   1.30476 -0.99674 -2.65552
C   0.24757 -0.52526 -1.88666
N  -0.66787 -0.10998 -2.84187
C  -0.19971 -0.31930 -4.14235
C   1.03970 -0.87115 -4.02390
C  -1.96115  0.48848 -2.59608
C  -2.12710  1.86708 -2.86644
C  -3.40453  2.42587 -2.67680
C  -4.49894  1.65348 -2.24923
C  -4.29760  0.27784 -2.02960
C  -3.04292 -0.33524 -2.20395
Ni  0.00996 -0.52882  0.01231
B   0.00482  1.37924 -0.03980
O   1.05866  2.21684 -0.53213
C   0.65027  3.52650 -0.37171
C  -0.64001  3.54055  0.18366
C  -1.31725  4.73093  0.44515
C  -0.64105  5.92898  0.12635
C   0.65342  5.91510 -0.42735
C   1.32832  4.70262 -0.68963
O  -1.04892  2.24067  0.40908
C  -0.99088  2.72598 -3.37954
C  -5.85536  2.28736 -2.02251
C  -2.88032 -1.82543 -2.02115
C   3.57525  0.65686 -1.83720
C   6.23485 -3.60122 -1.12442
C   1.48889 -3.89287 -2.87241
C  -0.24599 -0.41248  1.90501
N  -1.31425 -0.84091  2.68392
C  -1.06793 -0.64000  4.04688
C   0.16903 -0.08027  4.15169
N   0.65529  0.05815  2.84828
C  -2.53331 -1.50998  2.26786
C  -2.63340 -2.91002  2.46783
C  -3.84572 -3.53592  2.12812
C  -4.94836 -2.81665  1.63123
C  -4.82680 -1.42186  1.51000
C  -3.63659 -0.74092  1.83436
C   1.95139  0.64552  2.58912
C   3.04197 -0.19657  2.26546
C   4.29800  0.40855  2.07594
C   4.49286  1.79571  2.21580
C   3.39000  2.58845  2.57833
C   2.11084  2.03773  2.78159
C  -1.49556 -3.71840  3.04672
C  -6.22878 -3.52816  1.24769
C  -3.58217  0.76616  1.76617
C   2.88618 -1.69562  2.17163
C   5.85233  2.41774  1.97503
C   0.96849  2.92203  3.23462
Cl  0.03474 -2.84612  0.08470
H  -2.32173  4.73203  0.87746
H  -1.13557  6.88700  0.31620
H   1.14916  6.86252 -0.66191
H   2.33301  4.68234 -1.12094
H  -1.79908 -0.91581  4.80185
H   0.75126  0.22653  5.01596
H  -3.92959 -4.62063  2.26722
H  -5.68906 -0.83360  1.17334
H  -0.59879 -3.61380  2.41155
H  -1.76797 -4.78474  3.09752
H  -1.23188 -3.38562  4.06654
H  -6.14432 -3.98625  0.24504
H  -7.08565 -2.83501  1.22205
H  -6.46621 -4.34217  1.95347
H  -3.19144  1.19470  2.70604
H  -4.58973  1.17837  1.59606
H  -2.92021  1.12229  0.96167
H   5.15137 -0.23187  1.82297
H   3.52359  3.66846  2.71390
H   2.21231 -1.99139  1.34763
H   2.44613 -2.10824  3.09729
H   3.86394 -2.17597  2.01096
H   6.66734  1.73095  2.25844
H   5.97592  3.35296  2.54562
H   5.99293  2.66585  0.90673
H   0.84871  2.88915  4.33351
H   0.00748  2.61351  2.79560
H   1.15586  3.97022  2.95450
H   1.76106 -1.18679 -4.77268
H  -0.79480 -0.06180 -5.01398
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H	-3.54359	3.49573	-2.87355
H	-5.14417	-0.34785	-1.72303
H	-0.02867	2.45404	-2.91885
H	-1.18574	3.78958	-3.17209
H	-0.86827	2.61876	-4.47319
H	-5.96489	2.62871	-0.97650
H	-6.67345	1.57467	-2.21951
H	-6.00312	3.16839	-2.66876
H	-2.42211	-2.28863	-2.91312
H	-3.85819	-2.30125	-1.84835
H	-2.21915	-2.06845	-1.16990
H	5.68708	-0.90755	-1.17256
H	3.93158	-4.74704	-2.07276
H	3.19055	1.03646	-2.80046
H	4.58146	1.07824	-1.68220
H	2.90811	1.05445	-1.05678
H	6.50319	-4.40603	-1.83010
H	6.13765	-4.06796	-0.12711
H	7.07743	-2.89204	-1.07721
H	0.60722	-3.77965	-2.21796
H	1.77494	-4.95659	-2.89582
H	1.19345	-3.59716	-3.89466

Int(1-8)1

SCF = -2426.52395716
H(0 K)= -2425.650146
H(298 K)= -2425.590337
G(298 K)= -2425.748375
SCF(D3BJ) = -2426.81648028
SCF(BS2) = -3764.84066345
SCF(BS2+D3BJ) = -3765.13318664
Low Freq. = 10.6114cm-1, 14.2589cm-1

Ni	-0.09372	0.03223	-0.18292
N	-0.46748	-0.27740	2.72153
N	1.44328	0.65673	2.29342
N	-1.39519	-1.63567	-2.28042
N	0.59870	-2.41117	-1.97007
C	0.34232	0.08834	1.63807
C	0.11077	0.05043	3.95672
H	-0.38681	-0.17118	4.89725
C	1.31058	0.63287	3.68642
H	2.08192	1.02865	4.34183
C	-1.69663	-1.03152	2.69194
C	-1.61634	-2.44249	2.77446
C	-2.81153	-3.16929	2.92368
H	-2.75839	-4.26269	2.99633
C	-4.06387	-2.53048	3.00036
C	-4.10119	-1.12665	2.91508
H	-5.06665	-0.61027	2.98278
C	-2.93392	-0.35219	2.76775
C	-0.27704	-3.14150	2.73660
H	0.34045	-2.87641	3.61388
H	0.29752	-2.84084	1.84363
H	-0.40424	-4.23564	2.72739
C	-5.33778	-3.33574	3.14977
H	-5.16985	-4.25245	3.73944
H	-5.73012	-3.65178	2.16512
H	-6.13090	-2.74992	3.64305
C	-3.00443	1.15740	2.73427
H	-2.44568	1.60301	3.57694
H	-4.05015	1.49743	2.80286
H	-2.56348	1.56640	1.80941
C	2.62113	1.19995	1.66779
C	3.65766	0.31492	1.29343
C	4.82131	0.86293	0.72566
H	5.63235	0.18603	0.43069
C	4.97760	2.25128	0.54581
C	3.94565	3.10060	0.98383
H	4.06297	4.18645	0.88223
C	2.76273	2.60117	1.56076
C	3.52849	-1.16653	1.55517
H	2.69189	-1.59889	0.98044
H	3.32265	-1.36226	2.62281
H	4.44986	-1.69802	1.27504
C	6.22302	2.81436	-0.10669
H	7.10673	2.18664	0.09735
H	6.43834	3.83649	0.24651
H	6.10806	2.86730	-1.20530
C	1.71123	3.54171	2.10403
H	1.84253	3.69398	3.19185
H	0.69461	3.14579	1.95671
H	1.77466	4.52820	1.61985
C	-0.28427	-1.46368	-1.45048
C	0.05674	-3.11358	-3.05571
H	0.62089	-3.87477	-3.58795
C	-1.20094	-2.62661	-3.24654
H	-1.97036	-2.88578	-3.96932
C	-2.59337	-0.82825	-2.27218
C	-2.68825	0.25789	-3.17477
C	-3.88438	0.99752	-3.18841
H	-3.96891	1.84675	-3.87734
C	-4.96971	0.67809	-2.35080
C	-4.84674	-0.43305	-1.49673
H	-5.69053	-0.71623	-0.85580
C	-3.67191	-1.20553	-1.44420
C	-1.54984	0.61325	-4.10478
H	-0.64279	0.88233	-3.53536
H	-1.82078	1.46884	-4.74327
H	-1.27865	-0.23273	-4.76086
C	-6.23016	1.51694	-2.36012
H	-7.11092	0.92861	-2.05359
H	-6.42868	1.93964	-3.35918
H	-6.14384	2.36721	-1.65884
C	-3.57264	-2.41618	-0.54856
H	-3.27368	-3.31479	-1.11676
H	-4.53808	-2.62104	-0.06125
H	-2.81722	-2.26657	0.24075
C	1.96501	-2.65942	-1.57807
C	2.96961	-1.73389	-1.94808
C	4.31024	-2.09228	-1.71610
H	5.09737	-1.38961	-2.01477
C	4.66785	-3.32076	-1.12963
C	3.63812	-4.20259	-0.75443
H	3.89398	-5.16225	-0.28859
C	2.28105	-3.89882	-0.97257
C	2.62171	-0.40470	-2.57414
H	1.94626	-0.52551	-3.43882
H	3.52942	0.12112	-2.90916
H	2.09222	0.23912	-1.84520

C	6.12009	-3.67108	-0.88101
H	6.78348	-3.18948	-1.61833
H	6.28691	-4.76002	-0.92756
H	6.44819	-3.33569	0.12062
C	1.20287	-4.88984	-0.58812
H	0.34027	-4.38650	-0.12205
H	1.59774	-5.63585	0.11989
H	0.81600	-5.43855	-1.46591
C	0.72040	5.36314	-1.17602
C	-0.00176	6.53363	-0.85083
H	0.42107	7.51027	-1.10834
C	-1.25069	6.46675	-0.20662
H	-1.78566	7.39189	0.03158
C	-1.83292	5.22626	0.13874
H	-2.80462	5.16408	0.63735
H	1.69139	5.40469	-1.67806
C	0.13822	4.14252	-0.83174
C	-1.11476	4.07638	-0.18849
O	-1.44973	2.75931	0.03146
O	0.62280	2.87250	-1.03276
B	-0.35892	1.96181	-0.48393
H	-0.66581	0.97135	-1.31859

TS(1-8)

SCF = -2426.46373588
H(0 K)= -2425.593966
H(298 K)= -2425.534122
G(298 K)= -2425.691998
SCF(D3BJ) = -2426.72168951
SCF(BS2) = -3764.74560247
SCF(BS2+D3BJ) = -3765.03240299
Low Freq. = -603.5269cm-1, 10.7795cm-1

Ni	0.33964	-0.07124	-0.06661
N	1.34777	-1.22795	-2.61395
N	-0.81866	-1.28108	-2.58970
N	1.20792	1.31735	2.44563
N	0.48584	-0.68961	2.84989
C	0.26581	-0.93482	-1.78606
C	0.94602	-1.73263	-3.85367
H	1.66300	-2.01978	-4.61853
C	-0.41788	-1.76564	-3.83834
H	-1.13629	-2.09326	-4.58508
C	2.74319	-1.11286	-2.26237
C	3.39170	-2.23285	-1.69179
C	4.77084	-2.13492	-1.43276
H	5.28621	-2.99645	-0.99053
C	5.50495	-0.97329	-1.74059
C	4.82497	0.10806	-2.33083
H	5.38297	1.01550	-2.59205
C	3.44510	0.06409	-2.60569
C	2.63326	-3.50807	-1.39827
H	2.22563	-3.95654	-2.32212
H	1.77532	-3.32060	-0.73011
H	3.29039	-4.25242	-0.92149
C	6.98521	-0.88861	-1.43188
H	7.15734	-0.60204	-0.37800
H	7.48722	-0.13607	-2.06186
H	7.48776	-1.85805	-1.58842
C	2.73363	1.23605	-3.23797
H	2.23994	0.95313	-4.18449
H	3.43695	2.05740	-3.44725
H	1.94711	1.60411	-2.55264
C	-2.21275	-1.19646	-2.22717
C	-2.76043	-2.17817	-1.37168
C	-4.13625	-2.10805	-1.08529
H	-4.57265	-2.86134	-0.41809
C	-4.96197	-1.10890	-1.63026
C	-4.38187	-0.16794	-2.50212
H	-5.00939	0.61572	-2.94318
C	-3.01280	-0.19101	-2.82169
C	-1.90101	-3.27228	-0.78488
H	-1.15598	-2.85516	-0.08391
H	-1.33862	-3.80898	-1.56935
H	-2.51704	-4.00218	-0.23722
C	-6.43243	-1.02961	-1.27949
H	-7.05669	-0.87941	-2.17730
H	-6.62861	-0.17668	-0.60479
H	-6.77774	-1.94459	-0.77118
C	-2.42365	0.83498	-3.76460
H	-2.07366	0.37883	-4.70790
H	-1.56071	1.34028	-3.30088
H	-3.17540	1.59884	-4.01778
C	0.72374	0.18515	1.79043
C	0.81215	-0.12446	4.08759
H	0.70397	-0.67370	5.01932
C	1.26362	1.13694	3.83098
H	1.62694	1.91677	4.49503
C	1.63838	2.55294	1.83420
C	0.78488	3.67685	1.89291
C	1.25039	4.88698	1.34483
H	0.59298	5.76446	1.37612
C	2.52515	4.99966	0.76212
C	3.35490	3.86234	0.75159
H	4.36078	3.93480	0.31973
C	2.93786	2.62946	1.28293
C	-0.57868	3.60181	2.54401
H	-1.12485	2.69420	2.24147
H	-1.18752	4.47862	2.27396
H	-0.50057	3.57636	3.64677
C	2.98656	6.30386	0.14594
H	2.52225	7.17296	0.64105
H	2.71473	6.35529	-0.92460
H	4.08189	6.41641	0.20915
C	3.84985	1.42676	1.26507
H	3.96444	0.98771	2.27195
H	4.84924	1.69859	0.89031
H	3.43096	0.64156	0.61032
C	0.05496	-2.06023	2.72564
C	-1.28626	-2.39177	3.02506
C	-1.65172	-3.75095	2.97843
H	-2.68800	-4.02291	3.21369
C	-0.73207	-4.76208	2.64448
C	0.59755	-4.38928	2.36757
H	1.33554	-5.16528	2.13019
C	1.01877	-3.04806	2.41310
C	-2.29471	-1.32733	3.39395
H	-2.00108	-0.79082	4.31405
H	-3.28556	-1.77682	3.56690
H	-2.38652	-0.57104	2.59514

C	-1.16170	-6.21249	2.57246
H	-2.02262	-6.41269	3.23139
H	-0.34230	-6.89185	2.86110
H	-1.46497	-6.48821	1.54552
C	2.46405	-2.67446	2.17445
H	2.56048	-1.97576	1.32412
H	3.07140	-3.56919	1.96567
H	2.89451	-2.16497	3.05517
C	-4.54611	2.27779	0.98142
C	-5.20320	3.40944	0.44859
H	-6.18648	3.68960	0.84068
C	-4.61693	4.18305	-0.57074
H	-5.15171	5.05538	-0.96071
C	-3.34905	3.85809	-1.10200
H	-2.88367	4.45543	-1.89149
H	-4.99205	1.67406	1.77727
C	-3.29646	1.96446	0.44729
C	-2.70916	2.73801	-0.57061
O	-1.48142	2.20440	-0.90114
O	-2.44090	0.93139	0.77969
B	-1.28586	1.04575	-0.07553
H	1.22589	1.08207	-0.56973

^{3}Int(1-8)1

SCF = -2426.48102018
H(0 K)= -2425.608220
H(298 K)= -2425.548331
G(298 K)= -2425.707400
SCF(D3BJ) = -2426.77121369
SCF(BS2) = -3764.79428365
SCF(BS2+D3BJ) = -3765.08447712
Low Freq. = 9.5387cm-1, 16.0086cm-1

Ni	0.08238	-0.25455	0.01751
N	-0.53353	-0.37792	2.94881
N	1.45968	0.41667	2.61642
N	-1.04446	-1.12474	-2.65541
N	1.09296	-1.49980	-2.50734
C	0.37009	-0.10702	1.92219
C	-0.02166	-0.02953	4.20398
H	-0.58879	-0.18426	5.11799
C	1.23077	0.46594	3.99421
H	1.98072	0.83964	4.68634
C	-1.79760	-1.07065	2.84079
C	-1.79358	-2.48188	2.73387
C	-3.03155	-3.15047	2.76049
H	-3.03906	-4.24460	2.68160
C	-4.24955	-2.46133	2.90332
C	-4.20819	-1.05970	3.02995
H	-5.14508	-0.50322	3.15517
C	-2.99926	-0.34119	3.01229
C	-0.50244	-3.25607	2.61024
H	0.18959	-3.02553	3.43946
H	0.02592	-2.99017	1.67515
H	-0.69383	-4.34093	2.61070
C	-5.57042	-3.20217	2.91658
H	-5.42777	-4.27946	3.10143
H	-6.09792	-3.09991	1.95033
H	-6.24769	-2.80795	3.69353
C	-2.99331	1.15899	3.20121
H	-2.58346	1.43842	4.18943
H	-4.01818	1.55860	3.14180
H	-2.37268	1.66248	2.44159
C	2.71307	0.86453	2.05689
C	3.72091	-0.09061	1.79606
C	4.97294	0.37605	1.35567
H	5.76656	-0.35458	1.16077
C	5.23533	1.74538	1.17049
C	4.20735	2.66395	1.45172
H	4.39591	3.73740	1.32775
C	2.94111	2.25301	1.90678
C	3.47521	-1.56639	2.01530
H	2.70103	-1.94768	1.32756
H	3.12176	-1.76801	3.04199
H	4.39601	-2.14520	1.84489
C	6.58339	2.22133	0.67090
H	7.37332	1.47774	0.86698
H	6.87914	3.17081	1.14800
H	6.56394	2.40160	-0.41986
C	1.88381	3.27122	2.26553
H	1.78321	3.37337	3.36225
H	0.89557	2.98342	1.87306
H	2.14848	4.26213	1.86382
C	0.03004	-0.97694	-1.76754
C	0.69146	-1.95041	-3.76881
H	1.39553	-2.38627	-4.47268
C	-0.64668	-1.71420	-3.86056
H	-1.35600	-1.92020	-4.65741
C	-2.43374	-0.81124	-2.41884
C	-3.04270	0.22695	-3.16516
C	-4.41519	0.46362	-2.96247
H	-4.89416	1.27378	-3.52598
C	-5.18326	-0.29735	-2.06274
C	-4.54964	-1.35078	-1.37710
H	-5.13549	-1.98050	-0.69671
C	-3.18421	-1.63709	-1.54806
C	-2.26771	1.05027	-4.17017
H	-1.31737	1.39926	-3.73888
H	-2.85491	1.93077	-4.47690
H	-2.03471	0.47353	-5.08402
C	-6.64707	0.01385	-1.83235
H	-7.20566	-0.88162	-1.51225
H	-7.12618	0.41042	-2.74322
H	-6.77190	0.77668	-1.04164
C	-2.54727	-2.81406	-0.85201
H	-2.09111	-3.50939	-1.57994
H	-3.28867	-3.36595	-0.25442
H	-1.73678	-2.47728	-0.17888
C	2.46178	-1.64172	-2.07873
C	3.35371	-0.55867	-2.24579
C	4.71518	-0.78364	-1.96849
H	5.42127	0.04399	-2.10466
C	5.19560	-2.03573	-1.54255
C	4.27086	-3.08392	-1.37270
H	4.62460	-4.06663	-1.03705
C	2.89982	-2.91213	-1.63443
C	2.86278	0.78519	-2.73128
H	2.40284	0.70774	-3.73268
H	3.69127	1.50836	-2.78722
H	2.08706	1.18637	-2.05485

C	6.66716	-2.25034	-1.25614
H	7.28949	-1.48004	-1.73987
H	7.00805	-3.23835	-1.60950
H	6.87691	-2.20908	-0.17084
C	1.92582	-4.05881	-1.47172
H	1.03112	-3.74188	-0.90914
H	2.39694	-4.90013	-0.93918
H	1.57019	-4.43457	-2.44839
C	-1.42916	4.57272	-2.16122
C	-1.72909	5.84398	-1.61879
H	-1.89061	6.68827	-2.29730
C	-1.82302	6.04226	-0.23047
H	-2.05698	7.03855	0.15912
C	-1.61761	4.97750	0.67777
H	-1.68850	5.12201	1.75992
H	-1.35604	4.41146	-3.24067
C	-1.23051	3.52463	-1.25961
C	-1.32089	3.72638	0.13470
O	-1.06135	2.55035	0.79109
O	-0.92067	2.21693	-1.52306
B	-0.76911	1.54640	-0.23758
H	-1.46171	0.44200	-0.06961

^{3}TS(1-8)

SCF = -2426.46840850
H(0 K)= -2425.598187
H(298 K)= -2425.538471
G(298 K)= -2425.696283
SCF(D3BJ) = -2426.75885729
SCF(BS2) = -3764.78269039
SCF(BS2+D3BJ) = -3765.07313919
Low Freq. = -122.1194cm-1, 13.3804cm-1

Ni	0.05275	-0.28562	-0.00725
N	0.61302	-1.27732	-2.75978
N	-1.37433	-0.41642	-2.68751
N	1.28440	-0.18734	2.73454
N	-0.74275	-0.95547	2.82006
C	-0.28899	-0.71195	-1.86521
C	0.10596	-1.32994	-4.06145
H	0.67858	-1.74776	-4.88534
C	-1.14552	-0.78922	-4.01523
H	-1.89342	-0.64404	-4.79012
C	1.90862	-1.83578	-2.44628
C	1.98861	-3.19724	-2.07511
C	3.26609	-3.75504	-1.88462
H	3.34192	-4.80990	-1.59311
C	4.44090	-3.00063	-2.06407
C	4.31476	-1.64781	-2.43204
H	5.21835	-1.04148	-2.56876
C	3.06159	-1.04167	-2.63599
C	0.73982	-4.02865	-1.88572
H	0.14187	-4.08301	-2.81308
H	0.08653	-3.58665	-1.11253
H	0.99472	-5.05661	-1.58305
C	5.80538	-3.63766	-1.89972
H	5.78738	-4.44773	-1.15179
H	6.56199	-2.89864	-1.58825
H	6.15645	-4.08109	-2.85020
C	2.94961	0.40858	-3.04258
H	2.50234	0.51483	-4.04767
H	3.94216	0.88594	-3.06124
H	2.30315	0.96178	-2.33950
C	-2.63224	0.16001	-2.27556
C	-3.55979	-0.65255	-1.58608
C	-4.80280	-0.08967	-1.24343
H	-5.52785	-0.71055	-0.70401
C	-5.14077	1.23375	-1.57875
C	-4.20236	1.99707	-2.29768
H	-4.45285	3.02525	-2.58618
C	-2.94545	1.48403	-2.66667
C	-3.24136	-2.08971	-1.24809
H	-2.45991	-2.14868	-0.47041
H	-2.86280	-2.63609	-2.12971
H	-4.13507	-2.61009	-0.87142
C	-6.47267	1.82725	-1.17027
H	-6.88194	2.48427	-1.95629
H	-6.37118	2.44205	-0.25702
H	-7.21699	1.04240	-0.95720
C	-1.98407	2.32407	-3.47817
H	-1.94822	1.99539	-4.53319
H	-0.96084	2.26162	-3.07524
H	-2.29719	3.38011	-3.47198
C	0.20466	-0.49966	1.90485
C	-0.27037	-0.92742	4.13601
H	-0.88120	-1.25190	4.97450
C	1.00258	-0.44312	4.07958
H	1.73685	-0.26656	4.86093
C	2.59266	0.29039	2.34483
C	2.95026	1.62501	2.64532
C	4.25779	2.04263	2.33026
H	4.54257	3.07971	2.54631
C	5.20183	1.17470	1.75474
C	4.81716	-0.15790	1.51210
H	5.54428	-0.85998	1.08649
C	3.52475	-0.62581	1.80345
C	1.98154	2.58005	3.30777
H	0.98265	2.51680	2.84863
H	2.34133	3.61732	3.21711
H	1.86832	2.36176	4.38608
C	6.59011	1.66017	1.39382
H	6.89113	2.52301	2.01081
H	6.63686	1.98245	0.33714
H	7.34356	0.86491	1.52373
C	3.14727	-2.06342	1.54649
H	2.71695	-2.53776	2.44644
H	4.02353	-2.64888	1.22774
H	2.38315	-2.11551	0.74975
C	-2.06111	-1.45744	2.51731
C	-3.15475	-0.56179	2.52493
C	-4.44305	-1.10169	2.35474
H	-5.30222	-0.42020	2.36449
C	-4.66001	-2.48333	2.19219
C	-3.54322	-3.33949	2.19183
H	-3.69269	-4.41930	2.06989
C	-2.23322	-2.85117	2.35237
C	-2.94778	0.91905	2.74317
H	-2.53665	1.12035	3.74916
H	-3.90089	1.46315	2.65102
H	-2.23046	1.33757	2.01676

C	-6.05976	-3.03022	2.00269
H	-6.38564	-2.94266	0.94933
H	-6.79490	-2.47982	2.61362
H	-6.11758	-4.09715	2.27381
C	-1.04656	-3.78913	2.36212
H	-0.30195	-3.49111	1.60329
H	-1.36266	-4.82388	2.15571
H	-0.52709	-3.77867	3.33703
C	-0.23246	5.09674	1.04275
C	0.10675	6.24907	0.29823
H	-0.01907	7.23634	0.75484
C	0.60231	6.15005	-1.01472
H	0.85762	7.06158	-1.56521
C	0.77655	4.89577	-1.64158
H	1.16221	4.81043	-2.66176
H	-0.61957	5.16408	2.06374
C	-0.05615	3.86376	0.41520
C	0.43676	3.76453	-0.89901
O	0.49486	2.43898	-1.26735
O	-0.31227	2.59755	0.90182
B	0.02329	1.65726	-0.14445
H	1.51876	0.13215	-0.18816

^{3}Int(1-8)2

SCF = -2426.46790968
H(0 K)= -2425.596419
H(298 K)= -2425.536487
G(298 K)= -2425.694876
SCF(D3BJ) = -2426.76079892
SCF(BS2) = -3764.78160170
SCF(BS2+D3BJ) = -3765.07449098
Low Freq. = 12.3844cm-1, 15.7060cm-1

Ni	-0.29588	-0.17209	0.05746
H	-0.25305	-1.69636	-0.15587
O	2.37744	1.32448	0.08566
O	2.51606	-0.67180	-1.08058
N	-1.42192	-0.11551	2.84359
N	0.60554	-0.87342	2.86172
N	-0.85065	1.36702	-2.48833
N	-1.32502	-0.74013	-2.69216
C	3.74052	-0.03641	-1.11993
C	3.65463	1.17821	-0.41447
C	4.74778	2.03724	-0.29832
H	4.67191	2.98121	0.24935
C	5.94975	1.63271	-0.92118
H	6.83069	2.27958	-0.85283
C	6.03537	0.41698	-1.62544
H	6.98117	0.13314	-2.09871
C	4.92172	-0.44539	-1.73881
H	4.97721	-1.39016	-2.28753
C	-0.34090	-0.33734	1.99464
C	-1.15444	-0.50114	4.16143
H	-1.89261	-0.40258	4.95329
C	0.12327	-0.97808	4.16972
H	0.73366	-1.38312	4.97257
C	-2.71122	0.40632	2.46062
C	-3.71311	-0.49874	2.03867
C	-4.99148	0.01923	1.76386
H	-5.77917	-0.67077	1.43762
C	-5.28999	1.38809	1.91254
C	-4.26738	2.25038	2.34785
H	-4.48326	3.31795	2.47685
C	-2.96809	1.78499	2.62779
C	-3.41809	-1.97525	1.90572
H	-2.59329	-2.15066	1.19174
H	-4.30758	-2.52298	1.55724
H	-3.10360	-2.41080	2.87101
C	-6.67414	1.91501	1.59674
H	-6.83113	1.99476	0.50544
H	-6.83356	2.91703	2.02715
H	-7.45991	1.24549	1.98627
C	-1.88126	2.72994	3.08892
H	-1.49018	2.44813	4.08241
H	-2.25976	3.76225	3.15088
H	-1.02427	2.71407	2.39346
C	1.94952	-1.30405	2.54324
C	2.16060	-2.63102	2.10477
C	3.48796	-3.04522	1.88809
H	3.66721	-4.06893	1.53729
C	4.58313	-2.19179	2.11174
C	4.32966	-0.89128	2.58734
H	5.17144	-0.21624	2.78205
C	3.02345	-0.42440	2.81747
C	1.00360	-3.57087	1.87266
H	0.35805	-3.17492	1.06393
H	0.37320	-3.67177	2.77429
H	1.36230	-4.57267	1.58743
C	5.99832	-2.64822	1.82856
H	6.07387	-3.74791	1.80980
H	6.70732	-2.26639	2.58280
H	6.33835	-2.27446	0.84552
C	2.78022	0.97840	3.32605
H	2.13509	0.98700	4.22160
H	2.28010	1.58205	2.54942
H	3.73256	1.46859	3.58351
C	-0.90504	0.18915	-1.74150
C	-1.51759	-0.15839	-3.94913
H	-1.85396	-0.73952	-4.80382
C	-1.21867	1.16649	-3.82187
H	-1.23959	1.97982	-4.54257
C	-0.46273	2.66405	-1.99118
C	0.80681	3.17735	-2.33983
C	1.14132	4.46807	-1.88945
H	2.12717	4.87424	-2.14626
C	0.25381	5.24391	-1.12250
C	-1.01221	4.70621	-0.82201
H	-1.72904	5.30701	-0.24879
C	-1.39715	3.42278	-1.24963
C	1.77339	2.38483	-3.19117
H	1.78738	1.32142	-2.90372
H	2.79502	2.78315	-3.09378
H	1.49815	2.42598	-4.26130
C	0.65525	6.61429	-0.61837
H	1.13567	6.54672	0.37525
H	-0.21840	7.27899	-0.51266
H	1.37719	7.09957	-1.29595
C	-2.77848	2.88528	-0.95655
H	-3.29640	2.58671	-1.88532
H	-3.39351	3.64272	-0.44641

H -2.73171 1.98918 -0.31384
C -1.62010 -2.13646 -2.46702
C -0.64478 -3.10821 -2.78485
C -0.99351 -4.46200 -2.62644
H -0.24461 -5.22727 -2.86482
C -2.26531 -4.85952 -2.17309
C -3.21523 -3.85924 -1.89460
H -4.22033 -4.14845 -1.56335
C -2.91940 -2.49183 -2.04207
C 0.72828 -2.71044 -3.27309
H 0.67330 -2.10307 -4.19431
H 1.33591 -3.60337 -3.49114
H 1.25594 -2.10349 -2.51658
C -2.59851 -6.32397 -1.97838
H -2.03533 -6.96353 -2.67828
H -3.67420 -6.51776 -2.12514
H -2.34372 -6.65807 -0.95553
C -3.96374 -1.43411 -1.76712
H -3.63532 -0.74676 -0.96823
H -4.91640 -1.89428 -1.46012
H -4.15673 -0.81442 -2.66123
B 1.62938 0.15719 -0.30917

8

SCF = -2426.52192370
H(0 K)= -2425.649127
H(298 K)= -2425.589510
G(298 K)= -2425.745718
SCF(D3BJ) = -2426.82033027
SCF(BS2) = -3764.83733882
SCF(BS2+D3BJ) = -
3765.13574549
Low Freq. = 16.1157cm-1,
17.0255cm-1

Ni 0.00213 -0.53530 0.00314
H 0.00926 -2.07804 0.00978
O -0.97730 2.28614 0.63105
O 0.95444 2.29133 -0.64110
N -1.02089 -1.13644 2.69167
N 0.94714 -0.22953 2.78233
N -0.94787 -0.25970 -2.77669
N 1.02542 -1.15481 -2.68210
C 0.57385 3.59399 -0.38912
C -0.60909 3.59079 0.37091
C -1.23299 4.77477 0.76422
H -2.15286 4.76243 1.35603
C -0.62158 5.98297 0.36304
H -1.07979 6.93469 0.65141
C 0.56368 5.98617 -0.39657
H 1.01284 6.94033 -0.69106
C 1.18657 4.78128 -0.78994
H 2.10661 4.77383 -1.38157
C -0.03086 -0.61255 1.87202
C -0.66341 -1.08080 4.04565
H -1.32327 -1.44977 4.82624
C 0.57546 -0.51685 4.10188
H 1.23043 -0.30008 4.94125
C -2.26294 -1.74084 2.26957
C -2.30508 -3.14362 2.08622
C -3.54565 -3.73074 1.78103
H -3.59182 -4.81741 1.63792
C -4.72380 -2.96715 1.66889
C -4.63879 -1.57766 1.87003
H -5.54833 -0.96833 1.80228
C -3.42132 -0.93816 2.17539
C -1.05517 -3.98235 2.21605
H -0.29962 -3.64429 1.48309
H -1.27626 -5.04683 2.03821
H -0.60198 -3.88769 3.21896
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H 3.73222 3.44739 2.73580
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H 6.21450 3.13145 2.34323
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H -2.30875 -1.99115 -0.80046
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H 5.55138 -0.93451 -1.79484
C 4.74853 -2.94225 -1.65517
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TS(1-11)
SCF = -2426.49332490
H(0 K)= -2425.620634
H(298 K)= -2425.561465
G(298 K)= -2425.716704
SCF(D3BJ) = -2426.79119955
SCF(BS2) = -3764.80768995
SCF(BS2+D3BJ) = -
3765.10556460
Low Freq. = -128.5325cm-1,
11.0927cm-1

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N -1.99912 2.52267 1.08736
N 0.01588 3.25942 0.74008
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H -3.30629 2.74161 -1.31290
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C 3.74631 3.28573 0.96885
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C 4.09094 4.17169 -0.06985
C 3.05875 4.67889 -0.88121
H 3.30713 5.35563 -1.70798
C 1.70931 4.34325 -0.66293
C 2.07789 2.00057 2.38297
H 1.31315 2.44210 3.04565
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H 1.66465 1.04293 2.01241

C	5.53043	4.58973	-0.28820
H	6.23070	3.77003	-0.05584
H	5.80119	5.43992	0.36512
H	5.70697	4.90935	-1.32846
C	0.62382	4.89966	-1.55925
H	-0.07661	4.10792	-1.87396
H	1.06079	5.35884	-2.46021
H	0.02027	5.67159	-1.04883
C	2.96888	-3.14154	2.67979
C	2.96757	-4.46119	3.19357
H	3.81201	-4.79668	3.80509
C	1.90351	-5.33990	2.93579
H	1.92399	-6.35411	3.34847
C	0.79449	-4.93630	2.15297
H	-0.03907	-5.61460	1.94658
H	3.79599	-2.45118	2.86932
C	1.87086	-2.74623	1.91424
C	0.79903	-3.63297	1.65577
O	-0.14739	-3.02567	0.87311
O	1.65404	-1.54082	1.30866
B	0.29665	-1.60907	0.70244
H	-0.54572	-0.88035	1.35881

Int(1-11)1

SCF = -2426.50544226
H(0 K)= -2425.631535
H(298 K)= -2425.571912
G(298 K)= -2425.730210
SCF(D3BJ) = -2426.79182756
SCF(BS2) = -3764.82137940
SCF(BS2+D3BJ) = -3765.10776470
Low Freq. = 7.5418cm-1, 17.4464cm-1

Ni	-0.51618	0.77643	0.16494
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N	1.50880	-2.30965	-1.68458
N	-1.84919	3.25854	0.54428
N	0.27176	3.63438	0.24676
C	0.34025	-2.13397	-0.98997
C	-0.10004	-3.05627	-3.02067
H	-0.72512	-3.46233	-3.81101
C	1.25124	-2.86766	-2.93803
H	2.05293	-3.06918	-3.64294
C	-2.06831	-2.66378	-1.53670
C	-2.87692	-1.56538	-1.90550
C	-4.26312	-1.68146	-1.67844
H	-4.90747	-0.83553	-1.94383
C	-4.83488	-2.83921	-1.12453
C	-3.98667	-3.91275	-0.78539
H	-4.41610	-4.82481	-0.35388
C	-2.59657	-3.85054	-0.97885
C	-2.28042	-0.30458	-2.46631
H	-1.55272	-0.50388	-3.27133
H	-1.72541	0.25302	-1.65582
H	-3.06325	0.36478	-2.85532
C	-6.32672	-2.93666	-0.88533
H	-6.86867	-2.10884	-1.37003
H	-6.55841	-2.90248	0.19468
H	-6.73663	-3.88645	-1.27077
C	-1.70126	-5.00173	-0.58265
H	-1.06645	-5.34141	-1.41997
H	-2.29936	-5.85963	-0.23799
H	-1.03126	-4.68799	0.23696
C	2.85499	-1.97091	-1.26229
C	3.32578	-0.66732	-1.52203
C	4.66227	-0.38551	-1.18265
H	5.04562	0.62377	-1.37085
C	5.50678	-1.35388	-0.60988
C	4.98726	-2.64065	-0.36969
H	5.63060	-3.40657	0.07980
C	3.65872	-2.97703	-0.68457
C	2.42332	0.38586	-2.11416
H	1.56787	0.60838	-1.43363
H	1.98933	0.06298	-3.07752
H	2.97077	1.32686	-2.27525
C	6.93495	-1.01775	-0.23478
H	7.30025	-0.13585	-0.78595
H	7.61727	-1.85936	-0.44244
H	7.01989	-0.79219	0.84414
C	3.11283	-4.35644	-0.38860
H	2.65447	-4.82286	-1.27800
H	2.33396	-4.31429	0.39322
H	3.91309	-5.02131	-0.02839
C	-0.65724	2.58674	0.24688
C	-0.32449	4.86776	0.54365
H	0.25651	5.78375	0.61168
C	-1.65399	4.63061	0.73185
H	-2.47043	5.29837	0.99468
C	-3.14871	2.64134	0.64448
C	-3.51991	1.98656	1.84418
C	-4.82479	1.47377	1.93732
H	-5.12199	0.96192	2.86083
C	-5.75659	1.60280	0.88818
C	-5.35088	2.26437	-0.28451
H	-6.06310	2.37938	-1.11123
C	-4.05421	2.79402	-0.43012
C	-2.53698	1.82950	2.97943
H	-1.66717	1.23132	2.64171
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H	-2.14183	2.80440	3.31585
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H	-7.14209	-0.06922	0.99747
C	-3.64347	3.49958	-1.70383
H	-3.44399	4.57302	-1.53590
H	-4.43339	3.41955	-2.46776
H	-2.71410	3.06644	-2.11327
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C	2.54056	2.99842	0.98443
C	3.92557	3.01846	0.73973
H	4.59727	2.61110	1.50504
C	4.47137	3.55724	-0.44155
C	3.58712	4.06186	-1.41269
H	3.99040	4.47282	-2.34656
C	2.19193	4.05938	-1.22112
C	1.98707	2.41885	2.26317
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H	1.43207	1.48541	2.04734

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C   5.97147  3.62066 -0.64339
H   6.46812  2.70273 -0.28527
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H   6.23239  3.76121 -1.70519
C   1.26638  4.59483 -2.29225
H   0.43671  3.89320 -2.48350
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H   0.80731  5.55691 -2.00230
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C   2.52010 -2.56210  4.34880
H   3.31522 -2.50600  5.09995
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H   1.45703 -4.13973  5.38588
C   0.43117 -3.57907  3.55569
H  -0.39051 -4.29232  3.67369
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C   1.53783 -1.79757  2.29125
C   0.47974 -2.72349  2.45331
O  -0.40884 -2.63950  1.41716
O   1.38011 -1.07428  1.13693
B   0.11409 -1.54332  0.51401
H  -0.90379 -0.72531  0.47967
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Bcat_rad

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SCF  =       -406.343900055
H(0 K)=      -406.254825
H(298 K)=    -406.247807
G(298 K)=    -406.285700
SCF(D3BJ) = -406.365820098
SCF(BS2) = -406.500832222
SCF(BS2+D3BJ) = -
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Low Freq. = 225.6107cm-1,
234.2133cm-1

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C  -2.05042 -0.70444  0.00001
H  -3.00398 -1.24123  0.00001
C  -2.05041  0.70443  0.00001
H  -3.00395  1.24124  0.00002
C  -0.84892  1.44366  0.00002
H  -0.83766  2.53657  0.00002
H  -0.83762 -2.53658 -0.00001
C   0.32965 -0.70185 -0.00001
C   0.32971  0.70188  0.00001
O   1.65250  1.16105 -0.00002
O   1.65251 -1.16105  0.00001
B   2.41581 -0.00003 -0.00001
```

References

1 X. Bantreil and S. P. Nolan, *Nat. Protoc.*, 2011, **6**, 69–77.

2 A. J. Arduengo, S. F. Camper, J. C. Calabrese and F. Davidson, *J. Am. Chem. Soc.*, 1994, **116**, 4391–4394.

3 W. B. Reid, J. J. Spillane, S. B. Krause and D. A. Watson, *J. Am. Chem. Soc.*, 2016, **138**, 5539–5542.

4 J. A. Bailey, M. Ploeger and P. G. Pringle, *Inorg. Chem.*, 2014, **53**, 7763–7769.

5 N. Iwadate and M. Suginome, *J. Organomet. Chem.*, 2009, **694**, 1713–1717.

6 O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, *J. Appl. Cryst.*, 2009, **42**, 339–341.

7 G. M. Sheldrick, *Acta Cryst.*, 2008, **A64**, 112–122.

8 G. M. Sheldrick, *Acta Cryst.*, 2015, **C71**, 3–8.

9 G. M. Sheldrick, *Acta Cryst.*, 2015, **A71**, 3–8.

10 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian 09, Revision D.01, Gaussian, Inc., Wallingford CT, 2009.

11 A. D. Becke, *Phys. Rev. A*, 1988, **38**, 3098-3100.

12 J. P. Perdew, *Phys. Rev. B*, 1986, **33**, 8822-8824.

13 D. Andrae, U. Häußermann, M. Dolg, H. Stoll and H. Preuß, *Theor. Chim. Acta*, 1990, **77**, 123-141.

14 A. Höllwarth, M. Böhme, S. Dapprich, A. W. Ehlers, A. Gobbi, V. Jonas, K. F. Köhler, R. Stegmann, A. Veldkamp and G. Frenking, *Chem. Phys. Lett.*, 1993, **208**, 237-240.

15 P. C. Hariharan and J. A. Pople, *Theor. Chim. Acta*, 1973, **28**, 213-222.

16 J. Tomasi, B. Mennucci and R. Cammi, *Chem. Rev.*, 2005, **105**, 2999-3094.

17 F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys.*, 2005, **7**, 3297-3305.

18 S. Grimme, S. Ehrlich and L. Goerigk, *J. Comput. Chem.*, 2011, **32**, 1456-1465.

19 L. Tendera, T. Schaub, M. J. Krahfuss, M. W. Kuntze-Fechner and U. Radius, *Eur. J. Inorg. Chem.*, 2020, 3194